STIC Search Report
EIC 1700

STIC Database Tracking Number: 201968

TO: Eisa Elhilo
Location: REM 9C19
Art Unit : 1751
September 19, 2006

Case Serial Number: 10/525300

From: Mei Huang
Location: EIC 1700
REMSEN 4B28
Phone: 571/272-3952
Mei.huang@uspto.gov

Search Notes

Examiner Elhilo,

- 48 answers in total on combination of diazonium compd's and coupling agent.
- Zero hit on the coupling component (i), see L61, page 2 (L49-59 are some of the diazonium compounds that applicant didn't want to have for the coupling component (i).

Please feel free to contact me if you have any questions or if you would like to refine the search query,

Thank you for using STIC services!

Mei Huang

STIC Search Results Feedback Form

EIC17000

Questions about the scope or the results of the search? Contact ***the EIC searcher or contact:***

Kathleen Fuller, EIC 1700 Team Leader
571/272-2505 REMSEN 4B28

Voluntary Results Feedback Form

➢ *I am an examiner in Workgroup:* ☐ *Example: 1713*

➢ *Relevant prior art* ***found****, search results used as follows:*

- ☐ 102 rejection
- ☐ 103 rejection
- ☐ Cited as being of interest.
- ☐ Helped examiner better understand the invention.
- ☐ Helped examiner better understand the state of the art in their technology.

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature
  (journal articles, conference proceedings, new product announcements etc.)

➢ *Relevant prior art* ***not found:***

- ☐ Results verified the lack of relevant prior art (helped determine patentability).
- ☐ Results were not useful in determining patentability or understanding the invention.

Comments:

Drop off or send completed forms to EIC1700 REMSEN 4B28

```
=> fil reg
FILE 'REGISTRY' ENTERED AT 15:00:31 ON 19 SEP 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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=> d his

     (FILE 'HOME' ENTERED AT 10:05:39 ON 19 SEP 2006)

     FILE 'HCAPLUS' ENTERED AT 10:06:18 ON 19 SEP 2006
                E US20050251932/PN
L1            1 S E3
                SEL RN

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L2           64 S E1-64
L3              STR
L4           50 S L3
L5              STR
L6              STR L3
L7           50 S L6
L8           50 S L5
L9         7825 S L6 FUL
                SAV L9 ELH300F1/A
L10        3778 S L5 FUL
                SAV L10 ELH300F4/A
L11          37 S L2 AND L9
L12           0 S L2 AND L10
L13             STR
L14          27 S L2 NOT L11
L15           1 S 90-20-0/RN
L16           1 S 87-02-5/RN
L17           1 S 90-51-7/RN
L18           1 S 88-63-1/RN
L19           1 S 591-27-5/RN
L20           1 S 108-46-3/RN
L21           1 S 16867-03-1/RN
L22           1 S 31643-63-7/RN
                E 2(1H)-PYRIDINONE, 4-METHYL-6-HYDROXY-1-METHYL-/CN
L23           1 S 457629-66-2/RN
                E C7H9NO2/MF
L24           1 S 119-79-9/RN
L25           1 S 81-05-0/RN
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L27           1 S 6362-18-1/RN
L28           1 S 90-40-4/RN
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L33        2075 S L9(L)BIOL/RL
L34        3626 S L10
L35           0 S L10 (L) COS/RL
L36        1798 S L10 (L) BIOL/RL
L37        1759 S L15
L38        1496 S L16 OR L17
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L39         19667 S L18 OR L19 OR L20
L40           800 S L21
L41            28 S L22 OR L23
L42           567 S L24 OR L25
L43           761 S L26 OR L27
L44           130 S L28
L45            61 S L29
L46           164 S L30
L47            63 S (L31 OR L34) AND L37-L46
L48            48 S L47 AND (1840-2002)/PY,PRY

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L52             1 S 457629-59-3/RN
L53             1 S 67599-13-7/RN
L54             1 S 667878-10-6/RN
L55             1 S 457629-58-2/RN
L56             1 S 457629-65-1/RN
L57             1 S 667878-44-6/RN
L58             1 S 667878-45-7/RN
L59             1 S 30221-20-6/RN

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L61             0 S L48 AND L37 NOT L60
L62       1185415 S COLOR? OR COLOUR? OR PIGMENT? OR DYE? OR CHROMA# OR CHR
L63        165604 S HAIR? OR KERATIN? OR POROUS?(2N)MATERIAL?
L64            17 S L48 AND L62
L65             6 S L64 AND L63
L66            11 S L64 NOT L65
L67            31 S L48 NOT (L65 OR L66)


     FILE 'REGISTRY' ENTERED AT 15:00:31 ON 19 SEP 2006

=> d l9 que stat
L6                STR
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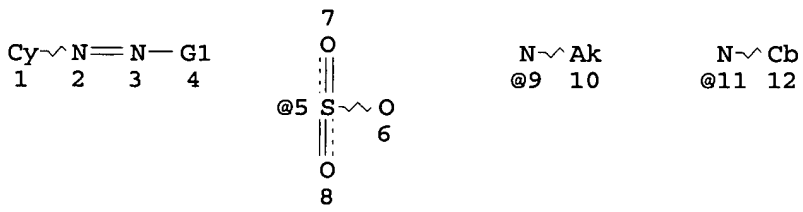


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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  12
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STEREO ATTRIBUTES: NONE
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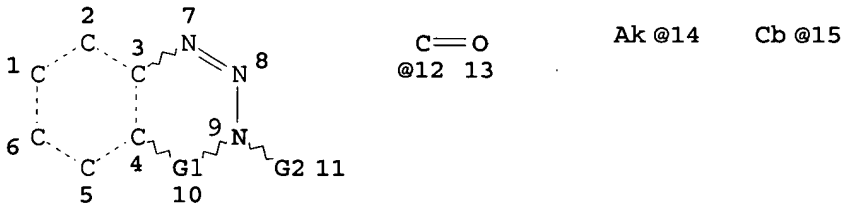

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VAR G2=14/15
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GGCAT IS SAT AT 14
GGCAT IS UNS AT 15
DEFAULT ECLEVEL IS LIMITED

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RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE
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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

=> d l65 ibib abs hitstr hitind 1-6

L65 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:167936 HCAPLUS
DOCUMENT NUMBER: 144:254145
TITLE: Preparation of novel pyrazolopyrimidines as cyclin dependent kinase inhibitors
INVENTOR(S): Guzi, Timothy J.; Paruch, Kamil; Dwyer, Michael P.
PATENT ASSIGNEE(S): Schering Corporation, USA
SOURCE: U.S. Pat. Appl. Publ., 85 pp., Cont.-in-part of U.S. Ser. No. 653,776.
CODEN: USXXCO

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006041131	A1	20060223	US 2005-244772	200510 06
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US 2004106624	A1	20040603	US 2003-653776	200309 03
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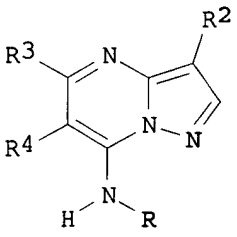
US 7067661	B2	20060627		
US 2006178371	A1	20060810	US 2006-395676	200603 31
			<--	
PRIORITY APPLN. INFO.:			US 2002-408029P P	200209 04
			<--	
			US 2003-653776 A2	200309 03

OTHER SOURCE(S): MARPAT 144:254145
GI



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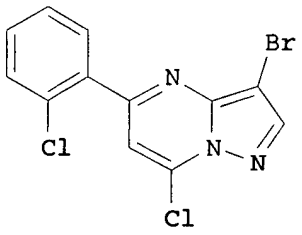

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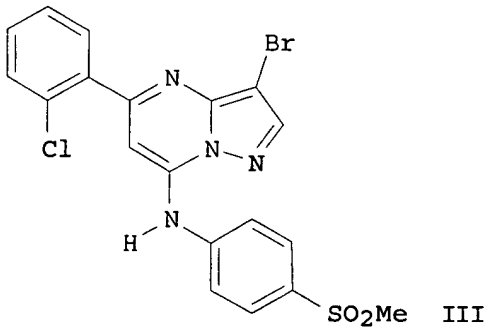


III

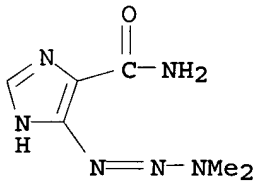
AB The title compds. I [R = aryl optionally substituted with one or

more heteroaryl; R2 = alkyl, cycloalkyl, CF3, etc.; R3 = H, halo, alkyl, etc.; R4 = H, halo, alkyl], useful as inhibitors of cyclin dependent kinases, were prepd. Thus, reacting II (prepn. given) with 4-methylsulfonylaniline hydrochloride in the presence of iPr2NEt afforded 23% III. The compds. I were tested in in vitro cyclin E/CDK2 kinase assay (biol. data given for representative compds. I). The invention also provides pharmaceutical compns. contg. one or more compds. I, methods of prepg. pharmaceutical formulations comprising one or more such compds., and methods of treatment, prevention, inhibition, or amelioration of one or more diseases assocd. with the CDKs using such compds. or pharmaceutical compns.

IT **4342-03-4**, Dacarbazine
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(prepn. of novel pyrazolopyrimidines as cyclin dependent kinase inhibitors for treatment and prevention of diseases)

RN 4342-03-4 HCAPLUS

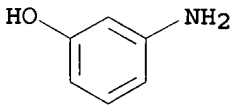
CN 1H-Imidazole-4-carboxamide, 5-(3,3-dimethyl-1-triazenyl)- (9CI) (CA INDEX NAME)



IT **591-27-5**, 3-Hydroxyaniline
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of novel pyrazolopyrimidines as cyclin dependent kinase inhibitors for treatment and prevention of diseases)

RN 591-27-5 HCAPLUS

CN Phenol, 3-amino- (9CI) (CA INDEX NAME)



INCL 544281000; 514252160; 514259300

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

IT Acute lymphocytic leukemia
Acute myeloid leukemia
Acute promyelocytic leukemia
Antitumor agents
Bladder, neoplasm
Chronic myeloid leukemia
Combination chemotherapy
Esophagus, neoplasm
Gallbladder, neoplasm
Hairy cell leukemia
Head and Neck, neoplasm
Hodgkin's disease

Human
Kidney, neoplasm
Leukemia
Liver, neoplasm
Lung, neoplasm
Mammary gland, neoplasm
Melanoma
Multiple myeloma
Myelodysplastic syndromes
Neuroglia, neoplasm
Ovary, neoplasm
Pancreas, neoplasm
Prostate gland, neoplasm
Radiotherapy
Skin, neoplasm
Stomach, neoplasm
(prepn. of novel pyrazolopyrimidines as cyclin dependent kinase inhibitors for treatment and prevention of diseases)

IT Skin, disease
(xeroderma **pigmentosum**; prepn. of novel pyrazolopyrimidines as cyclin dependent kinase inhibitors for treatment and prevention of diseases)

IT 50-07-7, Mitomycin-C 50-18-0, Cyclophosphamide 50-24-8, Prednisolone 50-44-2, 6-Mercaptopurine 50-76-0, Dactinomycin 50-91-9, Floxuridine 51-18-3, Triethylenemelamine 51-21-8, 5-Fluorouracil 51-75-2, Chlormethine 52-24-4, Thiotepa 53-03-2, Prednisone 53-19-0, Mitotane 54-91-1, Pipobroman 55-98-1, Busulfan 56-53-1, Diethylstilbestrol 57-22-7, Vincristine 57-63-6, 17-Ethinylestradiol 58-05-9, Leucovorin 58-18-4, Methyltestosterone 58-22-0, Testosterone 59-05-2, Methotrexate 66-75-1, Uracil mustard 68-96-2, Hydroxyprogesterone 71-58-9, Medroxyprogesteroneacetate 76-43-7, Fluoxymesterone 83-43-2, Methylprednisolone 124-94-7, Triamcinolone 125-84-8, Aminoglutethimide 127-07-1, Hydroxyurea 147-94-4, Ara-C 148-82-3, Melphalan 154-42-7, 6-Thioguanine 154-93-8, Carmustine 305-03-3, Chlorambucil 521-12-0, Dromostanolone propionate 569-57-3, Chlorotrianisene 595-33-5, Megestrolacetate 645-05-6, Hexamethylmelamine 671-16-9, Procarbazine 865-21-4, Vinblastine 968-93-4, Testolactone 1327-53-3, Trisenox 2998-57-4, Estramustine 3778-73-2, Ifosfamide **4342-03-4**, Dacarbazine 9015-68-3, L-Asparaginase 10540-29-1, Tamoxifen 11056-06-7, Bleomycin 13010-47-4, Lomustine 13311-84-7, Flutamide 14769-73-4, Levamisole 15663-27-1, Cisplatin 18378-89-7, Mithramycin 18883-66-4, Streptozocin 20830-81-3, Daunorubicin 23214-92-8, Doxorubicin 25316-40-9, Adriamycin 29767-20-2, Teniposide 33069-62-4, Taxol 33419-42-0, Etoposide 41575-94-4, Carboplatin 51264-14-3, Amsacrine 53643-48-4, Vindesine 53714-56-0, Leuprolide 53910-25-1, Pentostatin 56420-45-2, Epirubicin 58957-92-9, Idarubicin 61825-94-3, Oxaliplatin 65271-80-9, Mitoxantrone 65807-02-5, Goserelin 68335-15-9, Porfimer 71486-22-1, Vinorelbine 75607-67-9, Fludarabine phosphate 82413-20-5, Droloxifene 84449-90-1, Raloxifene 85622-93-1, Temozolomide 89778-26-7, Toremifene 95058-81-4, Gemcitabine 97682-44-5, Irinotecan 107868-30-4, Exemestane 112809-51-5, Letrazole 114977-28-5, Taxotere 120511-73-1, Anastrozole 123948-87-8, Topotecan 125317-39-7, Navelbine 129453-61-8, Fulvestrant 154361-50-9, Capecitabine 174722-31-7, Rituximab 179324-69-7, Velcade 180288-69-1, Herceptin 183319-69-9, Tarceva 184475-35-2, Iressa 192185-68-5, R115777 192391-48-3, Bexxar

193275-84-2, SCH 66336 195987-41-8, BMS 214662 205923-56-4, Erbitux 206181-63-7, Zevalin 216503-57-0, Campath 216974-75-3, Avastin 220127-57-1, Gleevec 253863-00-2, L778123
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(prepn. of novel pyrazolopyrimidines as cyclin dependent kinase inhibitors for treatment and prevention of diseases)

IT 62-53-3, Aniline, reactions 78-96-6 94-02-0, Ethyl benzoylacetate 100-46-9, Benzylamine, reactions 105-53-3, Diethyl malonate 107-10-8, Propylamine, reactions 108-00-9, N,N-Dimethylethylenediamine 108-42-9, 3-Chloroaniline 108-91-8, Cyclohexylamine, reactions 109-01-3, 1-Methylpiperazine 109-55-7, N,N-Dimethylpropylenediamine 109-85-3, 2-Methoxyethylamine 111-42-2, Bis(2-hydroxyethyl)amine, reactions 115-69-5 121-47-1, 3-Aminobenzenesulfonic acid 141-78-6, Ethyl acetate, reactions 156-87-6, 3-Hydroxypropylamine 504-24-5, 4-Aminopyridine **591-27-5**, 3-Hydroxyaniline 616-34-2, Methyl 2-aminoacetate 933-88-0, 2-Methylbenzoyl chloride 1003-03-8, Cyclopentylamine 1820-80-0, 3-Aminopyrazole 2038-03-1, 2-Morpholinoethylamine 2221-00-3 2524-67-6, 4-Morpholinoaniline 2719-27-9, Cyclohexanecarbonyl chloride 2836-04-6 2905-60-4, 2,3-Dichlorobenzoyl chloride 3182-95-4 3535-37-3, 3,4-Dimethoxybenzoyl chloride 3731-51-9, 2-(Aminomethyl)pyridine 3731-52-0, 3-(Aminomethyl)pyridine 5036-48-6, 1H-Imidazole-1-propanamine 5267-64-1 5271-67-0, 2-Thiophenecarbonyl chloride 5292-21-7, Cyclohexaneacetic acid 5470-49-5, 4-Methylsulfonylaniline 6168-72-5, 2-Aminopropanol 6575-24-2 7065-46-5 7663-77-6 10314-99-5 16617-46-2, 3-Amino-4-cyanopyrazole 21615-34-9, 2-Methoxybenzoyl chloride 23356-96-9, L-Prolinol 26116-12-1 51387-90-7 53369-71-4 58347-49-2 84358-12-3 87120-72-7, 1-tert-Butoxycarbonyl-4-aminopiperidine 89951-56-4 147081-44-5 147081-49-0 177662-76-9, 4-Methylsulfonylaniline hydrochloride 189017-89-8 216502-94-2 672323-27-2 672324-36-6 672325-00-7 672325-01-8 672325-02-9 672325-03-0 672325-04-1 672325-05-2 672325-06-3 672325-07-4 672325-08-5 672325-09-6 672325-10-9 672325-11-0 672325-12-1 672325-13-2 672325-19-8 672325-24-5 672325-38-1 673475-71-3 761446-44-0 877173-97-2 877173-98-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of novel pyrazolopyrimidines as cyclin dependent kinase inhibitors for treatment and prevention of diseases)

L65 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:100738 HCAPLUS
DOCUMENT NUMBER: 144:198849
TITLE: Novel dosage form comprising modified-release and immediate-release active ingredients
INVENTOR(S): Vaya, Navin; Karan, Rajesh Singh; Sadanand, Sunil; Gupta, Vinod Kumar
PATENT ASSIGNEE(S): India
SOURCE: U.S. Pat. Appl. Publ., 49 pp., Cont.-in-part of U.S. Ser. No. 630,446.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

US 2006024365	A1	20060202	US 2005-134633	200505 19
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IN 193042	A	20040626	IN 2002-MU697	200208 05
US 2004096499	A1	20040520	US 2003-630446	200307 29
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PRIORITY APPLN. INFO.:			IN 2002-MU697 A	200208 05
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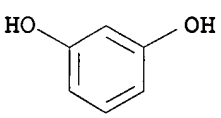
			IN 2002-MU699 A	200208 05
			<--	
			IN 2003-MU80 A	200301 22
			IN 2003-MU82 A	200301 22
			US 2003-630446 A2	200307 29

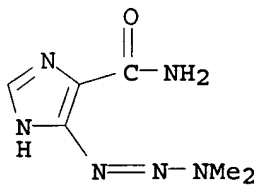
AB A dosage form comprising of a high dose, high soly. active ingredient as modified release and a low dose active ingredient as immediate release where the wt. ratio of immediate release active ingredient and modified release active ingredient is from 1:10 to 1:15000 and the wt. of modified release active ingredient per unit is from 500 mg to 1500 mg; a process for prepg. the dosage form. Tablets contg. 10 mg sodium pravastatin and 1000 mg niacin were prepd. The release of sodium pravastatin after 24 h was 67.7%, and the release of niacin after 1 h was 84.1%.

IT **108-46-3**, Resorcinol, biological studies **4342-03-4**, Dacarbazine
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel dosage form comprising modified-release and immediate-release active ingredients)

RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



RN 4342-03-4 HCAPLUS
CN 1H-Imidazole-4-carboxamide, 5-(3,3-dimethyl-1-triazenyl)- (9CI) (CA INDEX NAME)



INCL 424468000
CC 63-6 (Pharmaceuticals)
IT **Hair** preparations
(growth stimulants; novel dosage form comprising modified-release and immediate-release active ingredients)
IT **Dyes**
(tellurapyrylium; novel dosage form comprising modified-release and immediate-release active ingredients)
IT 85-79-0, Dibucaine 86-13-5, Benztropine 86-34-0, Phensuximide 86-35-1, Ethotoin 86-42-0, Amodiaquine 87-08-1, Penicillin V 87-90-1, Symclosene 89-25-8, Edaravone 89-57-6, Mesalamine 90-01-7, Salicyl alcohol 90-03-9, Mercufenol chloride 90-33-5, Hymecromone 90-86-8, Cinnamedrine 91-33-8, Benzthiazide 92-13-7, Pilocarpine 93-23-2, Lauryl isoquinolinium bromide 94-09-7, Benzocaine 94-12-2, Risocaine 94-14-4, Isobutamben 94-20-2, Chloropropamide 94-24-6, Tetracaine 94-25-7, Butamben 94-36-0, Benzoyl peroxide, biological studies 95-25-0, Chlorzoxazone 96-82-2 96-83-3, Iopanoic acid 97-24-5, Fenticlor 97-53-0, Eugenol 97-77-8, Disulfiram 98-72-6, Nitarsone 98-96-4, Pyrazinamide 99-66-1, Valproic acid 99-79-6, Iophendylate 100-33-4, Pentamidine 100-55-0, Nicotinyl alcohol 100-97-0, Methenamine, biological studies 101-26-8, Pyridostigmine bromide 101-31-5, Hyoscyamine 101-40-6, Propylhexedrine 102-71-6, Trolamine, biological studies 102-76-1, Triacetin 103-90-2, Paracetamol 104-31-4, Benzonatate 106-48-9 **108-46-3**, Resorcinol, biological studies 110-85-0, Piperazine, biological studies 112-24-3, Trientine 112-38-9, Undecylenic acid 112-72-1, 1-Tetradecanol 112-92-5, Stearyl [alcohol;] 113-18-8, Ethchlorvynol 113-52-0, Imipramine hydrochloride 113-59-7, Chlorprothixene 113-79-1D, Argipressin, hcompds. with tannate 113-92-8, Chlorpheniramine maleate 113-98-4, Penicillingpotassium 114-07-8, Erythromycin 114-49-8, Scopolamine hydrobromide 114-70-5, Sodium phenylacetate 114-80-7, Neostigmine bromide 114-85-2, Bethanidine sulfate 114-86-3, Phenformin 114-90-9, Obidoxime chloride 115-02-6, Azaserine 115-38-8, Mephobarbital 116-38-1, Edrophonium chloride 117-96-4, Diatrizoic acid 118-68-3, Etryptamine acetate 120-29-6D, Tropine, esters 120-97-8, Dichlorphenamide 121-19-7, Roxarsone 121-54-0, Benzethonium chloride 121-81-3, Nitromide 122-09-8, Phentermine 122-16-7, Sulfanitran 122-18-9, Cetalkonium chloride 122-32-7D, Triolein, iodo derivs., iodine-125 and iodine 131 122-79-2, Phenylacetate 123-03-5, Cetylpyridinium chloride 123-63-7, Paraldehyde 123-99-9, Azelaic acid, biological studies 124-07-2, Octanoic acid, biological studies 124-43-6, Carbamide peroxide 124-72-1, Teflurane 124-94-7, Triamcinolone 125-33-7, Primidone 125-40-6, Butabarbital 125-45-1, Azetepa 125-71-3, Dextromethorphan 125-72-4, Levorphanol tartrate 126-07-8, Griseofulvin 126-22-7, Butonate 126-27-2, Oxethazaine 127-07-1, Hydroxyurea 127-33-3, Demeclocycline 127-48-0, Trimethadione 127-69-5, Sulfisoxazole

127-71-9, Sulfabenzamide 127-77-5, Sulfabenz 127-79-7, Sulfamerazine 128-13-2, Ursodiol 128-62-1, Noscapine 129-06-6, Coumadin 129-20-4, Oxyphenbutazone 129-49-7, Methysergide maleate 129-51-1, Ergonovine maleate 129-74-8, Buclizine hydrochloride 130-16-5, Cloxyquin 130-26-7, Clioquinol 130-81-4, Quindonium bromide 131-49-7, Diatrizoate meglumine 132-17-2, Benztropine mesylate 132-35-4, Proxazole citrate 132-65-0, Dibenzothiophene 132-69-4, Benzydamine hydrochloride 132-92-3, Methicillin sodium 132-98-9, Penicillinvpotassium 133-11-9, Phenyl aminosalicylate 133-58-4, Nitromersol 133-67-5, Trichlormethiazide 134-80-5, Diethylpropion hydrochloride 135-07-9, Methyclothiazide 135-09-1, Hydroflumethiazide 136-40-3, Phenazopyridine hydrochloride 136-77-6, Hexylresorcinol 137-26-8, Thiram 137-53-1, Dextrothyroxine sodium 137-58-6, Lidocaine 138-39-6, Mafenide 143-67-9, Vinblastine sulfate 143-71-5, Hydrocodone bitartrate 144-14-9, Anileridine 144-80-9, Sulfacetamide 144-82-1, Sulfamethizole 145-63-1, Suramin 146-22-5, Nitrazepam 146-54-3, Triflupromazine 147-85-3, Proline, biological studies 147-94-4, Cytarabine 148-79-8, Thiabendazole 148-82-3, Melphalan 149-32-6, Erythritol 151-67-7, Halothane 152-11-4, Verapamil hydrochloride 152-43-2, Quinestrol 152-47-6, Sulfalene 152-58-9, Cortodoxone 152-97-6, Fluocortolone 153-87-7, Oxypertine 154-21-2, Lincomycin 154-41-6, Phenylpropanolamine hydrochloride 154-42-7, Thioguanine 154-68-7, Antazoline phosphate 154-69-8, Tripelennamine hydrochloride 154-93-8, Carmustine 156-51-4, Phenelzine sulfate 271-95-4, 1,2-Benzisoxazole 297-76-7, Ethynodiol diacetate 298-46-4, Carbamazepine 298-57-7, Cinnarizine 298-59-9, Methylphenidate hydrochloride 299-39-8, Sparteine sulfate 299-42-3, Ephedrine 302-22-7, Chlormadinone acetate 302-49-8, Uredepa 302-79-4, Tretinoin 303-53-7, Cyclobenzaprine 304-20-1, Hydralazine hydrochloride 304-55-2, Succimer 304-84-7, Ethamivan 305-03-3, Chlorambucil 306-07-0, Pargyline hydrochloride 306-21-8, Hydroxyamphetamine hydrobromide 309-36-4, Methohexital sodium 314-19-2, Apomorphine hydrochloride 315-80-0, Dibenzepin hydrochloride 316-42-7, Emetine hydrochloride 317-52-2, Hexafluorenium bromide 318-98-9, Propranolol hydrochloride 319-89-1, Tetroquinone 320-67-2, Azacitidine 322-35-0, Benserazide 326-43-2, Phenyramidol hydrochloride 329-65-7, Racepinephrine 333-36-8, Flurothyl 338-98-7, Isoflupredone acetate 339-72-0, Levcycloserine 340-57-8, Mecloqualone 345-78-8, Pseudoephedrine hydrochloride 346-18-9, Polythiazide 356-12-7, Fluocinonide 357-07-3, Oxymorphone hydrochloride 357-70-0, Galantamine 359-83-1, Pentazocine 361-37-5, Methysergide 362-29-8, Propiomazine 363-20-2, Tricetamide 363-24-6, Dinoprostone 364-62-5, Metoclopramide 364-98-7, Diazoxide 366-70-1, Procarbazine hydrochloride 378-44-9, Betamethasone 379-79-3, Ergotamine tartrate 382-67-2, Desoximetasone 389-08-2, Nalidixic acid 390-64-7, Prenylamine 396-01-0, Triamterene 404-82-0, Fenfluramine hydrochloride 404-86-4, Capsaicin 406-90-6, Fluroxene 423-55-2, Perflubron 424-89-5, Clomegestone acetate 426-13-1, Fluorometholone 434-05-9, Methenolone acetate 434-07-1, Oxymetholone 435-97-2, Phenprocoumon 437-74-1, Xanthinol niacinate 439-14-5, Diazepam 440-17-5, Trifluoperazine hydrochloride 443-48-1, Metronidazole 446-86-6, Azathioprine 451-71-8, Glyhexamide 459-86-9, Mitoguazone 465-65-6, Naloxone 466-06-8, Proscillaridin 467-22-1, Carbiphene hydrochloride 472-15-1, Betulinic acid 474-25-9, Chenodiol 474-58-8, Sitogluside 474-86-2, Equilin 476-70-0, Boldine 480-30-8, Dichloralphenazone 480-39-7,

Pinocembrin 483-63-6, Crotamiton 486-56-6, Cotinine 486-66-8, Daidzein 501-75-7
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel dosage form comprising modified-release and immediate-release active ingredients)

IT 1524-88-5, Flurandrenolide 1538-09-6 1553-34-0, Methixene hydrochloride 1553-60-2, Ibufenac 1597-82-6, Paramethasone acetate 1605-68-1, Taxane 1605-89-6, Bolasterone 1607-17-6, Pentrinitrol 1622-61-3, Clonazepam 1622-62-4, Flunitrazepam 1639-60-7, Propoxyphene hydrochloride 1642-54-2, Diethylcarbamazine citrate 1649-18-9, Azaperone 1661-29-6, Meturedepa 1665-48-1, Metaxalone 1684-40-8, Tacrine hydrochloride 1707-14-8, Phenmetrazine hydrochloride 1722-62-9, Mepivacaine hydrochloride 1740-22-3, Pyrinoline 1744-22-5, Riluzole 1764-85-8, Epithiazide 1786-81-8, Prilocaine hydrochloride 1808-12-4, Bromodiphenhydramine hydrochloride 1812-30-2, Bromazepam 1841-19-6, Fluspirilene 1847-63-8, Nafoxidine hydrochloride 1866-43-9, Rolodine 1867-66-9, Ketamine hydrochloride 1892-80-4, Fenethylline hydrochloride 1893-33-0, Pipamperone 1910-68-5, Methisazone 1977-10-2, Loxapine 1977-11-3, Perlapine 1980-45-6, Benzodepa 1982-37-2, Methdilazine 1986-53-4, Bolandiol dipropionate 2013-58-3, Meclocycline 2022-85-7, Flucytosine 2030-63-9, Clofazimine 2056-56-6, Cintazone 2058-52-8, Clothiapine 2062-78-4, Pimozide 2062-84-2, Benperidol 2068-78-2, Vincristine sulfate 2078-54-8, Propofol 2098-66-0, Cyproterone 2109-73-1, Butacetin 2119-75-7, Fluperolone acetate 2127-01-7, Clorexolone 2135-14-0, Descinolone acetonide 2135-17-3, Flumethasone 2152-34-3, Pemoline 2154-02-1, Methopholine 2167-85-3, Pipazethate 2169-64-4, Azaribine 2181-04-6, Canrenoate potassium 2210-77-7, Pyrrocaine 2218-68-0, Chloral betaine 2244-21-5, Troclosene potassium 2259-96-3, Cyclothiazide 2276-90-6, Iothalamic acid 2313-87-3, Ethoxazene hydrochloride 2315-02-8, Oxymetazoline hydrochloride 2321-07-5, Fluorescein 2324-94-9, Profadol hydrochloride 2353-33-5, Decitabine 2364-72-9, Cyprolidol hydrochloride 2391-03-9, Dexbrompheniramine maleate 2398-96-1, Tolnaftate 2438-32-6, Dexchlorpheniramine maleate 2441-88-5, Fenyripol hydrochloride 2447-57-6, Sulfadoxine 2465-59-0, Oxypurinol 2487-63-0, Quinbolone 2508-79-4, Methyldopate hydrochloride 2521-01-9, Encyprate 2529-45-5, Flurogestone acetate 2607-06-9, Diflucortolone 2608-24-4, Piposulfan 2612-33-1, Clonitrate 2618-25-9, Ioglycamic acid 2668-66-8, Medrysone 2687-96-9 2740-04-7, Dimefline hydrochloride 2750-76-7, Rifamide 2751-09-9, Troleandomycin 2753-45-9, Mebeverine hydrochloride 2768-90-3, Quinaldine blue 2809-21-4, Etidronic acid 2825-60-7, Formocortal 2829-19-8, Rolicyprine 2856-75-9, Modaline sulfate 2898-11-5, Medazepam hydrochloride 2898-13-7, Sulazepam 2919-66-6, Melengestrol acetate 2921-92-8, Propatyl nitrate 2955-38-6, Prazepam 2975-34-0, Carphenazine maleate 2988-32-1, Indriline hydrochloride 2998-57-4, Estramustine 3000-39-3, Quingestanol acetate 3044-32-4, Clogestone acetate 3056-17-5, Stavudine 3073-59-4, Hexamethylene bisacetamide 3093-35-4, Halcinonide 3105-97-3, Hycanthone 3115-05-7, Iobenzamic acid 3116-76-5, Dicloxacillin 3122-01-8, Thiazesim hydrochloride 3124-93-4, Ethynerone 3137-73-3, Anagestone acetate 3200-06-4, Nafronyl oxalate 3202-55-9, Benapryzine hydrochloride 3211-76-5, Selenomethionine 3239-45-0, Dexfenfluramine hydrochloride 3270-71-1, Nifuraldezone 3282-75-5, Ethanolamine oleate 3313-26-6, Thiothixene 3374-05-8, Nalidixate sodium 3385-03-3, Flunisolide 3416-26-0, Lidoflazine

3440-28-6, Betamipron 3459-20-9, Glymidine sodium 3485-14-1, Cyclacillin 3485-62-9, Clidinium bromide 3505-38-2, Carbinoxamine maleate 3511-16-8, Hetacillin 3521-84-4, Iodipamide meglumine 3538-57-6, Haloprogesterone 3546-41-6, Pyrvinium pamoate 3562-84-3, Benzbromarone 3570-10-3, Benorterone 3570-75-0, Nifurthiazole 3572-80-3, Cyclazocine 3577-01-3, Cephaloglycin 3599-32-4, Indocyanine green 3601-19-2, Ropizine 3614-69-5, Dimethindene maleate 3624-96-2, Bialamicol hydrochloride 3666-69-1, Dioxadrol hydrochloride 3688-85-5, Diapamide 3693-39-8, Flucloronide 3696-28-4, Dipyrithione 3704-09-4, Mibolerone 3715-90-0, Tramazoline hydrochloride 3717-88-2, Flavoxate hydrochloride 3734-16-5, Prodilidine hydrochloride 3735-90-8, Phencarbamide 3737-09-5, Disopyramide 3771-19-5, Nafenopin 3778-73-2, Ifosfamide 3784-99-4, Stilbazium iodide 3791-63-7 3795-88-8, Levofuraltadone 3810-74-0, Streptomycin sulfate 3810-80-8, Diphenoxylate hydrochloride 3819-00-9, Piperacetazine 3845-22-5, Teroxalene hydrochloride 3858-89-7, Chloroprocaine hydrochloride 3861-73-2, Anazolene sodium 3876-10-6, Clominorex 3930-19-6, Streptonigrin 3930-20-9, Sotalol 3978-86-7, Azatadine maleate 4015-32-1, Quazodine 4105-38-8 4117-65-1, Aspartocin 4171-13-5, Valnoctamide 4197-24-4, Carbol-Fuchsin 4205-90-7, Clonidine 4258-85-9, Clocortolone acetate 4268-36-4, Tybamate 4291-63-8, Cladribine 4320-13-2, Thiazinamium chloride 4330-99-8, Trimeprazine tartrate **4342-03-4**, Dacarbazine 4386-35-0, Meralein sodium 4434-20-2, Clothixamide maleate 4499-40-5, Oxtriphylline 4548-15-6, Flunidazole 4551-59-1, Fenalamide 4598-67-8 4663-83-6, Buramate 4682-36-4, Orphenadrine citrate 4724-59-8, Clamoxyquin hydrochloride 4759-48-2, Isotretinoin 4803-27-4, Anthramycin 4803-44-5, Levopropylcillin potassium 4803-45-6, Thiphencillin potassium 4936-47-4, Nifuratel 4991-68-8, Pimetine hydrochloride 5002-47-1, Fluphenazine decanoate 5034-76-4, Indoxole 5036-03-3, Nifurdazil 5051-62-7, Guanabenz 5053-06-5, Fenspiride 5055-20-9, Nifurquinazol 5055-42-5, Silandrone 5072-26-4, Buthionine sulfoximine 5086-74-8, Tetramisole hydrochloride 5090-37-9, Metizoline hydrochloride 5104-49-4, Flurbiprofen 5118-17-2, Furazolium chloride 5250-39-5, Floxacillin 5251-34-3, Cloprednol 5289-74-7, Ecdysterone 5318-76-3, Imidocarb hydrochloride 5322-53-2, Oxiperomide 5355-16-8, Diaveridine 5370-01-4, Mexiletine hydrochloride 5373-42-2, Thaliblastine 5467-78-7, Fenamole 5490-27-7, Dihydrostreptomycin sulfate 5508-58-7, Andrographolide 5522-33-8, Difluanine hydrochloride 5534-09-8, Beclomethasone dipropionate 5536-17-4, Vidarabine 5560-62-3, Biphenamine hydrochloride 5560-69-0, Ethyl dibunate 5560-72-5, Iprindole 5560-73-6, Mimbane hydrochloride 5560-75-8, Pyroxamine maleate 5560-77-0, Rotoxamine 5560-78-1, Teclozan 5578-73-4, Sanguinarium chloride 5579-13-5, Capuride 5579-16-8, Epinephryl borate 5579-27-1, Simtrazene 5579-85-1, Bromchlorenone 5579-92-0, Iopydol 5579-93-1, Iopydone 5579-94-2, Merisoprol Hg 197 5579-95-3, Nifurmerone 5581-35-1, Amphecloral 5581-40-8, Dimefadane 5581-42-0, Glyparamide 5581-46-4, Molinazone
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel dosage form comprising modified-release and immediate-release active ingredients)

L65 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:141200 HCAPLUS
DOCUMENT NUMBER: 142:254568
TITLE: Methods and compositions for increasing the

efficacy of biologically-active ingredients such as antitumor agents

INVENTOR(S): Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan M.; Thomas, Collin E.

PATENT ASSIGNEE(S): Board of Regents, the University of Texas System, USA

SOURCE: PCT Int. Appl., 243 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005014777	A2	20050217	WO 2003-US32667	200310 16
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WO 2005014777	A3	20050915		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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EP 1576150	A3	20051102		
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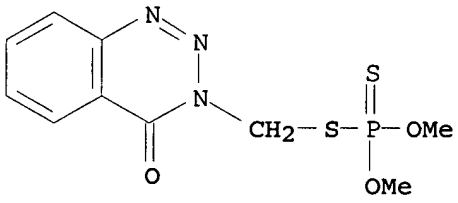
PRIORITY APPLN. INFO.:				
			US 2002-418803P	P 200210 16
			<--	
			WO 2003-US32667	W 200310 16

AB The invention provides methods and compns. for modulating the sensitivity of cells to cytotoxic compds. and other active agents. In accordance with the invention, compns. are provided comprising

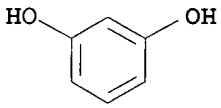
combinations of ectophosphatase inhibitors and active agents. Active agents include antibiotics, fungicides, herbicides, insecticides, chemotherapeutic agents, and plant growth regulators. By increasing the efficacy of active agents, the invention allows use of compns. with lowered concns. of active ingredients.

IT **86-50-0 108-46-3**, 1,3-Benzenediol, biological studies **961-22-8 2642-71-9 4342-03-4 24310-40-5 24310-41-6**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methods and compns. for increasing efficacy of biol. active ingredients such as antitumor agents)

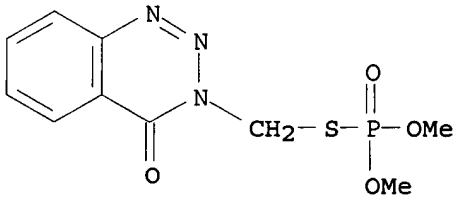
RN 86-50-0 HCAPLUS
CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



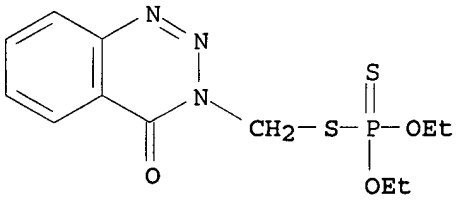
RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



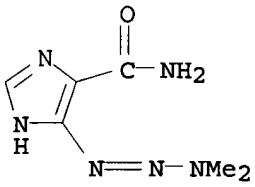
RN 961-22-8 HCAPLUS
CN Phosphorothioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (9CI) (CA INDEX NAME)



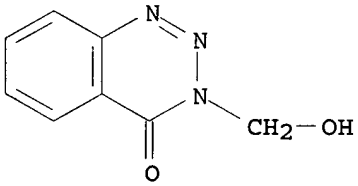
RN 2642-71-9 HCAPLUS
CN Phosphorodithioic acid, O,O-diethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



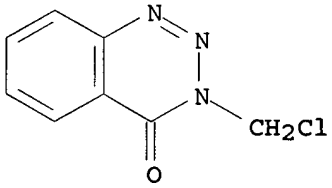
RN 4342-03-4 HCAPLUS
CN 1H-Imidazole-4-carboxamide, 5-(3,3-dimethyl-1-triazenyl)- (9CI) (CA INDEX NAME)



RN 24310-40-5 HCAPLUS
CN 1,2,3-Benzotriazin-4(3H)-one, 3-(hydroxymethyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 24310-41-6 HCAPLUS
CN 1,2,3-Benzotriazin-4(3H)-one, 3-(chloromethyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IC ICM C12N
CC 1-6 (Pharmacology)
IT **Pigments**, nonbiological
(cadmium yellow; methods and compns. for increasing efficacy of biol. active ingredients such as antitumor agents)
IT **Pigments**, nonbiological
(iron oxide; methods and compns. for increasing efficacy of biol. active ingredients such as antitumor agents)

IT **Dyes**
(liq., Green M; methods and compns. for increasing efficacy of biol. active ingredients such as antitumor agents)

IT Acacia
Acute lymphocytic leukemia
Adrenal cortex, neoplasm
Agrobacterium tumefaciens
Agrobacterium vitis
Agrotis segetum granulovirus
Alkylating agents, biological
Allium cepa
Allium sativum
Ampelomyces quisqualis
Anthracene oil
Antibiotic resistance
Apparatus
Arabidopsis thaliana
Arachis hypogaea
Aschersonia aleyrodis
Autographa californica nucleopolyhedrovirus
Avena sativa
Bacillus amyloliquefaciens
Bacillus cereus
Bacillus sphaericus
Bacillus subtilis
Bacillus thuringiensis
Bacillus thuringiensis darmstadiensis
Bacillus thuringiensis morrisoni
Beeswax
Bladder, neoplasm
Bone meal
Brain, neoplasm
Bran
Burkholderia cepacia
Capsicum
Caramel (**color**)
Carcinoid
Cheese
Chronic lymphocytic leukemia
Chronic myeloid leukemia
Cinnamon (horticultural common name)
Colloids
Combination chemotherapy
Cork
Corncob
Cottonseed meal
Creosote
Cytotoxic agents
Daucus carota
Desmodium
Drug delivery systems
Drug screening
Drugs
Dyes
Egg
Esophagus, neoplasm
Filter paper
Flours and Meals
Fumigants
Fungicides

Gentiana
Glues
Gossypium hirsutum
Hairy cell leukemia
Helicoverpa zea
Helicoverpa zea nucleopolyhedrovirus
Herbicides
Hodgkin's disease
Honey
Human
Insecticides
Jet aircraft fuel
Liliopsida
Lung, neoplasm
Lymantria dispar nucleopolyhedrovirus
Magnoliopsida
Mammary gland, neoplasm
Matricaria recutita
Meat
Medicago sativa
Melanoma
Mentha piperita
Milk
Mint
Molasses
Multiple myeloma
Neodiprion lecontii nucleopolyhedrovirus
Neodiprion sertifer
Nicotiana tabacum
Nosema locustae
Oatmeal
Odor and Odorous substances
Orgyia pseudotsugata nucleopolyhedrovirus
Oryza sativa
Ovary, neoplasm
Paecilomyces fumoso-roseus
Paecilomyces lilacinus
Paenibacillus lentimorbus
Paints
Paper
Paperboard
Peanut butter
Phlebia gigantea
Phlebiopsis gigantea
Phytophthora palmivora
Piper nigrum
Polycythemia vera
Propellants (sprays and foams)
Prostate gland, neoplasm
Pseudomonas chlororaphis
Pseudomonas fluorescens
Pseudomonas syringae
Puccinia canaliculata
Quassia
Quillaja
Rabbit calicivirus
Raisin
Rhizobium leguminosarum
Rhizobium leguminosarum phaseoli
Rosmarinus officinalis

Sawdust
Seaweed
Sinorhizobium meliloti
Skin, neoplasm
Sludges
Solanum tuberosum
Sorghum bicolor
Soybean meal
Sphagnum
Spodoptera exigua nucleopolyhedrovirus
Staphylococcus aureus
Stomach, neoplasm
Streptomyces griseoviridis
Tar oils
Testis, neoplasm
Thickening agents
Thymus (plant)
Tomato mosaic virus
Trichoderma harzianum
Trichoderma polysporum
Trigonella foenum-graecum
Triticum aestivum
Urogenital system, disease
Verticillium lecanii
Wheat flour
Whey
Wool
Xanthomonas campestris poannua
Yeast
Zea mays
(methods and compns. for increasing efficacy of biol. active ingredients such as antitumor agents)

IT **Dyes**
(water-sol.; methods and compns. for increasing efficacy of biol. active ingredients such as antitumor agents)

IT **Pigments**, nonbiological
(yellow, cadmium; methods and compns. for increasing efficacy of biol. active ingredients such as antitumor agents)

IT 50-00-0, Formaldehyde, biological studies 50-07-7 50-18-0 50-29-3, biological studies 50-44-2 50-70-4, D-Glucitol, biological studies 50-76-0, Actinomycin D 50-79-3 50-91-9 50-99-7, D-Glucose, biological studies 51-21-8 51-28-5, biological studies 51-36-5 52-24-4 52-68-6 52-85-7 52-90-4, L-Cysteine, biological studies 53-03-2 53-19-0 53-41-8 54-11-5 54-64-8 55-38-9 55-68-5 55-98-1 56-23-5, biological studies 56-35-9 56-36-0 56-38-2 56-53-1 56-72-4 56-75-7 57-06-7 57-09-0 57-13-6, Urea, biological studies 57-22-7 57-48-7, D-Fructose, biological studies 57-50-1, biological studies 57-63-6 57-85-2 58-27-5 58-36-6 58-89-9 59-05-2 59-30-3D, analogs, biological studies 59-50-7 59-87-0 60-00-4, biological studies 60-12-8, Benzeneethanol 60-51-5 60-57-1 61-73-4 62-38-4 62-53-3, Benzenamine, biological studies 62-73-7 62-76-0 63-25-2 63-42-3 64-00-6 64-02-8 64-17-5, Ethanol, biological studies 65-30-5 66-25-1, Hexanal 66-81-9 67-48-1 67-56-1, Methanol, biological studies 67-63-0, 2-Propanol, biological studies 67-64-1, 2-Propanone, biological studies 67-66-3, biological studies 67-68-5, biological studies 67-72-1 69-72-7, biological studies 70-30-4 70-38-2 70-43-9 71-23-8, 1-Propanol, biological studies 71-36-3, 1-Butanol, biological studies 71-55-6 71-58-9 71-63-6 72-20-8 72-43-5

72-54-8 72-55-9, biological studies 74-82-8D, Methane, triaryl derivs. 74-83-9, biological studies 74-85-1, Ethene, biological studies 74-87-3, biological studies 74-88-4, biological studies 74-90-8, Hydrocyanic acid, biological studies 74-96-4 74-98-6, Propane, biological studies 75-00-3 75-05-8, Acetonitrile, biological studies 75-07-0, Acetaldehyde, biological studies 75-08-1, Ethanethiol 75-09-2, biological studies 75-15-0, Carbon disulfide, biological studies 75-20-7, Calcium carbide (Ca(C2)) 75-21-8, Oxirane, biological studies 75-28-5 75-31-0, 2-Propanamine, biological studies 75-35-4, biological studies 75-37-6 75-43-4 75-45-6 75-52-5, biological studies 75-56-9, biological studies 75-60-5 75-68-3 75-69-4 75-71-8 75-73-0 76-01-7 76-13-1 76-22-2 76-43-7 76-44-8 76-73-3 76-87-9 77-47-4 77-48-5 77-73-6 77-92-9D, copper complexes 77-98-5 78-21-7 78-34-2 78-40-0 78-48-8 78-53-5 78-57-9 78-70-6 78-78-4 78-83-1, biological studies 78-87-5 78-90-0D, 1,2-Propanediamine, 1-alkyl derivs., salts 78-92-2, 2-Butanol 78-93-3, 2-Butanone, biological studies 79-00-5 79-01-6, biological studies 79-08-3 79-09-4, Propanoic acid, biological studies 79-10-7, 2-Propenoic acid, biological studies 79-11-8, biological studies 79-21-0, Ethaneperoxoic acid 79-24-3 79-31-2 79-43-6, biological studies 79-46-9 80-05-7, biological studies 80-13-7 80-33-1 80-46-6 80-56-8 80-57-9 80-62-6 80-71-7 81-81-2 81-82-3 81-84-5, 1H,3H-Naphtho[1,8-cd]pyran-1,3-dione 81-88-9 82-66-6 82-68-8 83-26-1 83-28-3 83-79-4 84-62-8 84-66-2 84-74-2 85-00-7 85-34-7 85-68-7 85-86-9 85-97-2 **86-50-0** 86-85-1 86-86-2, 1-Naphthaleneacetamide 86-87-3, 1-Naphthaleneacetic acid 87-17-2 87-41-2, 1(3H)-Isobenzofuranone 87-44-5 87-47-8 87-51-4, 1H-Indole-3-acetic acid, biological studies 87-86-5 87-90-1 88-04-0 88-06-2 88-85-7 89-68-9 89-83-8 90-03-9 90-43-7, [1,1'-Biphenyl]-2-ol 91-44-1 91-64-5, 2H-1-Benzopyran-2-one 92-04-6 93-71-0 93-76-5 93-76-5D, alkylamine salts 93-78-7 93-79-8 93-80-1 94-13-3 94-26-8 94-43-9 94-59-7 94-62-2 94-75-7, biological studies 94-75-7D, alkylamine and alkanolamine salts 94-80-4 95-06-7 95-14-7, 1H-Benzotriazole 95-48-7, biological studies 95-50-1 95-57-8 95-95-4 96-12-8 96-29-7 97-11-0 97-17-6 97-18-7 97-23-4 97-24-5 97-53-0 97-63-2 97-80-3 97-95-0 97-99-4 98-01-1, 2-Furancarboxaldehyde, biological studies 98-09-9, Benzenesulfonyl chloride 98-11-3D, Benzenesulfonic acid, C10-13-alkyl derivs., sodium salts 98-11-3D, Benzenesulfonic acid, alkyl derivs., potassium salts 98-11-3D, Benzenesulfonic acid, para-C9-13 alkyl derivs., sodium salts 98-50-0 98-54-4 98-82-8 98-86-2, biological studies
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
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IT 99-26-3 99-30-9 99-76-3 99-96-7, biological studies 100-00-5 100-41-4, biological studies 100-44-7, biological studies 100-51-6, Benzenemethanol, biological studies 100-56-1 100-57-2 100-94-7D, acylamido alkyl derivs. 100-95-8 101-05-3 101-20-2 101-21-3 101-42-8 101-81-5 101-84-8D, tetrapropylene derivs., sulfonated, sodium salts 102-07-8 102-30-7 102-71-6D, copper hydroxide complexes 103-11-7 103-27-5 104-28-9 104-54-1 104-55-2 104-60-9 104-76-7 105-67-9 106-22-9 106-23-0 106-24-1 106-44-5, biological studies 106-46-7 106-48-9 106-88-7 106-93-4 106-96-7 106-97-8, Butane, biological studies 106-99-0, 1,3-Butadiene, biological studies 107-04-0

107-06-2, biological studies 107-18-6, 2-Propen-1-ol, biological studies 107-19-7, 2-Propyn-1-ol 107-26-6 107-27-7 107-31-3 107-49-3 107-64-2 108-05-4, Acetic acid ethenyl ester, biological studies 108-07-6 108-11-2 108-24-7 108-31-6, 2,5-Furandione, biological studies 108-39-4, biological studies **108-46-3**, 1,3-Benzenediol, biological studies 108-80-5, 1,3,5-Triazine-2,4,6(1H,3H,5H)-trione 108-83-8 108-88-3, biological studies 108-90-7, biological studies 108-93-0, Cyclohexanol, biological studies 108-94-1, Cyclohexanone, biological studies 108-95-2, Phenol, biological studies 109-62-6 109-66-0, Pentane, biological studies 109-69-3 109-76-2D, 1,3-Propanediamine, N-C12-18alkyl derivs. 109-76-2D, 1,3-Propanediamine, N-C15-18alkyl derivs., diacetate 109-76-2D, 1,3-Propanediamine, N-C6-18alkyl derivs., acetate 109-76-2D, 1,3-Propanediamine, N-C6-18alkyl derivs., diacetate 109-76-2D, 1,3-Propanediamine, N-alkyl derivs. 109-76-2D, 1,3-Propanediamine, N-alkyl derivs. hydrochloride 109-76-2D, 1,3-Propanediamine, N-alkyl derivs., propionate-copper complex 109-76-2D, 1,3-Propanediamine, N-alkyl derivs., salts 109-76-2D, 1,3-Propanediamine, N-coco-alkyl derivs., adipate 109-76-2D, 1,3-Propanediamine, N-coco-alkyl derivs., hydroxyacetate 109-76-2D, 1,3-Propanediamine, N-coco-alkyl derivs., monobenzoate 109-79-5, 1-Butanethiol 109-94-4 109-99-9, biological studies 110-12-3 110-17-8, 2-Butenedioic acid (2E)-, biological studies 110-19-0 110-43-0, 2-Heptanone 110-54-3, Hexane, biological studies 110-66-7, 1-Pentanethiol 110-80-5 110-82-7, Cyclohexane, biological studies 110-88-3, 1,3,5-Trioxane, biological studies 111-01-3 111-20-6, Decanedioic acid, biological studies 111-27-3, 1-Hexanol, biological studies 111-70-6, 1-Heptanol 111-76-2 111-77-3 111-87-5, 1-Octanol, biological studies 111-90-0 111-98-8 112-02-7 112-05-0, Nonanoic acid 112-30-1, 1-Decanol 112-31-2, Decanal 112-34-5 112-44-7, Undecanal 112-53-8, 1-Dodecanol 112-54-9, Dodecanal 112-62-9 112-72-1, 1-Tetradecanol 112-92-5, 1-Octadecanol 113-98-4 114-26-1 115-07-1, 1-Propene, biological studies 115-10-6 115-28-6 115-29-7 115-31-1 115-32-2 115-90-2 115-93-5 116-01-8 116-02-9 116-06-3 116-16-5 116-25-6 116-52-9 117-52-2 117-81-7 117-84-0 118-34-3 118-52-5 118-56-9 118-74-1 119-12-0 119-38-0 120-23-0 120-32-1 120-39-8 120-47-8 120-72-9, 1H-Indole, biological studies 120-78-5 120-82-1 120-83-2 120-94-5 121-20-0 121-21-1 121-29-9 121-33-5 121-54-0 121-75-5 122-10-1 122-14-5 122-15-6 122-19-0 122-34-9 122-37-2 122-39-4, biological studies 122-42-9 122-64-5 122-70-3 122-97-4, Benzenepropanol 123-17-1 123-33-1 123-35-3 123-66-0 123-86-4 123-88-6 123-91-1, 1,4-Dioxane, biological studies 123-92-2 124-03-8 124-07-2, Octanoic acid, biological studies 124-13-0, Octanal 124-16-3 124-25-4, Tetradecanal 124-38-9, Carbon dioxide, biological studies 124-48-1 124-58-3 124-65-2 125-67-7 125-84-8 126-06-7 126-07-8 126-22-7 126-73-8, Phosphoric acid tributyl ester, biological studies 126-75-0 126-94-3 127-07-1 127-18-4, biological studies 127-41-3 127-82-2 128-03-0 128-04-1 128-37-0, biological studies 128-80-3 129-06-6 129-67-9 131-11-3 131-52-2 131-55-5 131-57-7 131-89-5 132-27-4 132-66-1 132-67-2 133-06-2 133-07-3 133-90-4 136-24-3 136-32-3 136-45-8 136-53-8 136-77-6 137-16-6 137-26-8 137-30-4 137-40-6 137-41-7 137-42-8 138-86-3 139-02-6 139-07-1 139-08-2 139-12-8 139-13-9 139-33-3 139-40-2 139-89-9 140-39-6 140-41-0 140-88-5 141-00-4 141-27-5 141-66-2 142-03-0 142-47-2 142-59-6

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RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
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IT 142-87-0 143-18-0 143-28-2 143-33-9, Sodium cyanide (Na(CN)) 143-50-0 144-21-8 144-41-2 144-55-8, Carbonic acid monosodium salt, biological studies 144-62-7, Ethanedioic acid, biological studies 145-73-3 145-73-3D, di-(N,N-dimethylcocoamine) salts 145-73-3D, mono- and di-(N,N-diethylalkylamine)and mono- and di-(N,N-dimethylalkylamine) salts 147-14-8 147-94-4 148-61-8 148-79-8 148-82-3 149-30-4, 2(3H)-Benzothiazolethione 149-57-5 150-38-9 150-39-0 150-50-5 150-68-5 150-84-5 151-21-3, biological studies 151-38-2 151-41-7D, salts 151-50-8, Potassium cyanide (K(CN)) 151-56-4D, Aziridine, derivs. 154-21-2 154-42-7 154-93-8 155-04-4 180-84-7, 1,7-Dioxaspiro[5.5]undecane 262-12-4D, Dibenzo[b,e][1,4]dioxin, chloro derivs. 288-88-0, 1H-1,2,4-Triazole 289-95-2D, Pyrimidine, analogs 290-87-9, 1,3,5-Triazine 297-97-2 298-00-0 298-01-1 298-02-2 298-03-3 298-04-4 298-06-6 298-14-6 299-84-3 300-76-5 301-04-2 301-12-2 302-01-2, Hydrazine, biological studies 305-03-3 309-00-2 311-45-5 314-40-9 314-42-1 315-18-4 317-83-9 319-84-6 319-85-7 327-98-0 328-04-1 329-21-5 330-54-1 330-55-2 330-64-3 333-20-0 333-40-4 333-41-5 333-43-7 334-48-5, Decanoic acid 338-45-4 352-93-2 379-52-2 404-86-4 443-48-1 465-73-6 470-90-6 471-34-1, Carbonic acid calcium salt (1:1), biological studies 475-26-3 485-31-4 497-19-8, Carbonic acid disodium salt, biological studies 499-75-2 500-28-7 502-39-6 506-87-6 507-60-8 509-34-2 512-42-5 513-77-9 513-78-0 513-92-8 515-42-4 515-83-3 517-16-8 518-47-8 525-79-1 526-18-1 527-07-1 527-09-3 533-96-0 534-16-7 534-52-1 540-72-7 540-73-8 541-31-1 542-75-6 544-60-5 546-93-0 548-62-9 554-13-2 555-37-3 556-61-6 557-05-1 557-41-5 563-12-2 563-47-3 563-63-3 569-64-2 571-58-4 572-48-5 578-94-9 580-48-3 584-08-7 584-79-2 588-66-9 590-28-3 592-01-8, Calcium cyanide (Ca(CN)2) 593-29-3 594-30-9 595-33-5 598-02-7 603-33-8 607-12-5 608-73-1 624-83-9 628-63-7 629-25-4 630-56-8 634-66-2 637-03-6 637-12-7 639-58-7 640-15-3 643-79-8, 1,2-Benzenedicarboxaldehyde 644-64-4 645-05-6 645-92-1 671-04-5 671-16-9 672-04-8 673-04-1 682-80-4 683-18-1 709-98-8 732-11-6 741-58-2 756-09-2 759-94-4 786-19-6 811-97-2 813-78-5 814-49-3 814-91-5 824-39-5 824-78-2 831-76-5 834-12-8 841-06-5 845-52-3 860-22-0 865-21-4, Vincaleukoblastine 867-27-6 872-50-4, biological studies 886-50-0 900-95-8 919-44-8 919-54-0 919-76-6 919-86-8 944-22-9 947-02-4 950-10-7 950-35-6 950-37-8 953-17-3 957-51-7 959-98-8 960-25-8 961-11-5 **961-22-8** 962-58-3 963-22-4 973-21-7 991-42-4 999-81-5 1007-28-9 1011-73-0 1014-69-3 1014-70-6 1024-57-3 1031-07-8 1066-30-4 1066-33-7 1066-45-1 1067-29-4 1071-83-6 1076-46-6 1079-33-0 1111-67-7 1111-78-0 1113-02-6 1113-38-8 1114-71-2 1129-41-5 1134-23-2 1136-84-1 1172-63-0 1184-57-2 1184-64-1 1186-49-8 1191-17-9 1191-50-0 1191-80-6 1193-18-6 1194-65-6 1300-34-1 1300-71-6 1300-72-7 1300-78-3 1301-96-8, Silver oxide (AgO) 1302-42-7 1303-28-2, Arsenic oxide (As2O5) 1303-33-9, Arsenic sulfide (As2S3) 1303-86-2, Boron oxide (B2O3), biological studies 1303-96-4, Borax (B4Na2O7.10H2O)
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

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IT 1305-62-0, Calcium hydroxide (Ca(OH)2), biological studies 1306-19-0, Cadmium oxide (CdO), biological studies 1306-23-6, Cadmium sulfide (CdS), biological studies 1308-38-9, Chromium oxide (Cr2O3), biological studies 1309-37-1, Iron oxide (Fe2O3), biological studies 1309-48-4, Magnesium oxide (MgO), biological studies 1310-58-3, Potassium hydroxide (K(OH)), biological studies 1310-65-2, Lithium hydroxide (Li(OH)) 1310-73-2, Sodium hydroxide (Na(OH)), biological studies 1312-76-1 1313-60-6, Sodium peroxide (Na2(O2)) 1313-82-2, Sodium sulfide (Na2S), biological studies 1314-13-2, Zinc oxide (ZnO), biological studies 1314-23-4, Zirconium oxide (ZrO2), biological studies 1314-80-3, Phosphorus sulfide (P2S5) 1314-84-7, Zinc phosphide (Zn3P2) 1317-36-8, Lead oxide (PbO), biological studies 1317-38-0, Copper oxide (CuO), biological studies 1317-39-1, Copper oxide (Cu2O), biological studies 1318-00-9, Vermiculite (Mg0.33[Mg2-3(Al0-1Fe0-1)0-1](Si2.33-3.33Al0.67-1.67)(OH)2O10.4H2O) 1319-53-5, Malachite (Cu2(CO3)(OH)2) 1319-77-3 1320-67-8 1320-79-2 1322-98-1 1323-19-9 1327-31-7, Lead arsenate hydroxide (Pb5(AsO4)3(OH)) 1327-43-1 1327-44-2 1327-53-3, Arsenic oxide (As2O3) 1328-53-6, C.I. **Pigment** Green 7 1330-16-1 1330-20-7, biological studies 1330-43-4, Boron sodium oxide (B4Na2O7) 1330-85-4 1332-40-7 1332-65-6, Copper chloride hydroxide (Cu2Cl(OH)3) 1332-77-0, Boron potassium oxide (B4K2O7) 1333-08-0 1333-16-0 1333-22-8, Copper hydroxide sulfate (Cu4(OH)6(SO4)) 1333-83-1, Sodium fluoride (Na(HF2)) 1334-75-4 1334-77-6 1335-30-4 1336-15-8, Calcium copper chloride oxide 1336-21-6, Ammonium hydroxide ((NH4)(OH)) 1340-69-8, Quaternium 18-bentonite 1343-88-0 1343-98-2, Silicic acid 1344-00-9 1344-08-7, Sodium sulfide (Na2(Sx)) 1344-09-8 1344-28-1, Aluminum oxide (Al2O3), biological studies 1344-43-0, Manganese oxide (MnO), biological studies 1344-67-8, Copper chloride 1344-72-5 1344-73-6 1344-74-7 1344-81-6, Calcium sulfide (Ca(Sx)) 1398-61-4, Chitin 1405-89-6, Bacitracin zinc 1420-07-1 1444-64-0 1454-85-9, 1-Heptadecanol 1461-22-9 1490-04-6 1491-41-4 1563-66-2 1570-64-5 1582-09-8 1594-56-5 1600-27-7 1610-17-9 1610-18-0 1634-78-2 1646-87-3 1646-88-4 1689-83-4 1689-84-5 1689-99-2 1701-93-5 1702-17-6 1746-01-6 1746-81-2 1754-58-1 1757-18-2 1762-95-4 1771-07-9 1776-83-6 1861-32-1 1861-40-1 1891-95-8 1897-45-6 1910-42-5 1912-24-9 1912-24-9D, dealkylated 1912-25-0 1912-26-1 1918-00-9 1918-02-1 1918-02-1D, alkanolamine salt 1918-08-7 1918-11-2 1918-13-4 1918-16-7 1918-18-9 1928-43-4 1928-45-6 1928-47-8 1928-48-9 1928-57-0 1928-58-1 1929-73-3 1929-77-7 1929-88-0 1934-21-0 1940-43-8 1954-81-0 1966-58-1 1967-16-4 1982-47-4 1982-49-6 1982-69-0 1983-10-4 1984-06-1 2008-39-1 2008-41-5 2008-46-0 2016-48-0 2032-59-9 2032-65-7 2050-99-9 2074-50-2 2082-79-3 2104-64-5 2104-96-3 2122-70-5 2155-70-6 2163-68-0 2163-69-1 2163-79-3 2163-80-6 2164-07-0 2164-08-1 2164-17-2 2173-56-0 2179-25-1 2212-54-6 2212-63-7 2212-67-1 2227-17-0 2235-25-8 2235-54-3 2244-21-5 2275-06-1 2275-14-1 2275-18-5 2275-23-2 2279-64-3 2280-44-6D, D-Glucopyranose, oligomeric, decyl octyl glycosides 2282-34-0 2300-66-5 2302-17-2 2303-17-5 2307-49-5 2310-17-0 2312-76-7 2321-53-1 2327-02-8 2353-45-9 2385-85-5 2402-95-1 2425-06-1 2425-10-7 2425-25-4 2425-66-3 2425-85-6

2439-00-1 2439-99-8 2440-22-4 2463-84-5 2465-65-8
2487-01-6 2492-26-4 2497-06-5 2497-07-6 2532-49-2
2536-26-7 2536-27-8 2540-82-1 2544-94-7 2545-59-7
2545-60-0 2577-72-2 2587-90-8 2588-03-6 2588-04-7
2588-05-8 2588-06-9 2591-21-1 2593-10-4 2593-15-9
2595-54-2 2597-03-7 2597-92-4 2597-93-5 2597-95-7
2597-97-9 2600-69-3 2610-86-8 2624-17-1 2631-37-0
2631-40-5 2635-10-1 2636-26-2 2637-34-5, 2(1H)-Pyridinethione
2642-71-9 2650-18-2 2655-14-3 2655-15-4 2655-19-8
2665-30-7 2668-92-0 2669-32-1 2674-91-1 2675-77-6
2682-20-4 2686-99-9 2689-43-2 2699-79-8, Sulfuryl fluoride
2701-86-2 2703-13-1 2759-71-9 2764-72-9 2778-04-3
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
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IT 2782-57-2 2782-70-9 2797-51-5 2809-21-4 2813-95-8
2875-41-4D, N-alkyl derivs. 2893-78-9 2905-69-3 2917-32-0
2921-88-2 2934-07-8 2939-80-2 2941-55-1 2953-29-9
2961-61-7 2961-62-8 2971-38-2 2991-51-7 3004-70-4
3032-40-4 3049-71-6 3050-27-9 3060-89-7 3097-08-3
3134-12-1 3134-70-1 3184-65-4 3247-34-5 3251-23-8
3279-27-4 3279-46-7 3282-00-6 3282-73-3 3304-97-0
3309-87-3 3337-71-1 3380-34-5 3383-96-8 3391-86-4,
1-Octen-3-ol 3397-62-4 3452-97-9 3478-94-2 3486-30-4
3486-35-9 3566-00-5 3566-10-7 3567-62-2 3568-56-7
3572-06-3 3583-63-9 3615-21-2 3626-13-9 3658-77-3
3689-24-5 3691-35-8 3724-65-0D, 2-Butenoic acid, esters
3734-49-4 3734-95-0 3734-97-2 3735-23-7 3735-33-9
3737-22-2 3740-92-9 3766-60-7 3766-81-2 3768-14-7
3772-94-9 3778-73-2 3792-59-4 3811-04-9 3811-49-2
3844-45-9 3861-41-4 3861-47-0 3878-19-1 3926-62-3
3960-05-2 4029-02-1 4075-81-4 4095-45-8 4097-34-1
4097-36-3 4147-51-7 4147-57-3 4154-35-2 4234-79-1
4342-03-4 4342-30-7 4342-36-3 4418-66-0 4419-22-1
4466-14-2 4476-04-4 4482-55-7 4489-31-0 4602-84-0
4636-83-3 4644-96-6 4654-26-6 4658-28-0 4665-55-8
4684-94-0 4685-14-7 4706-78-9 4719-04-4 4726-14-1
4808-30-4 4812-20-8 4824-78-6 4849-32-5 4938-72-1
5012-62-4 5026-62-0 5035-58-5 5064-31-3 5131-24-8
5131-66-8 5136-51-6 5137-55-3 5221-53-4 5234-68-4
5251-79-6 5251-93-4 5259-88-1 5281-04-9 5324-84-5
5328-04-1 5331-91-9 5335-24-0 5375-87-1 5386-57-2
5386-68-5 5386-77-6 5406-97-3 5468-43-9 5471-51-2
5538-94-3 5598-13-0 5598-15-2 5598-52-7 5716-15-4
5722-59-8 5723-62-6 5736-15-2 5742-19-8 5787-50-8
5822-97-9 5823-13-2 5826-76-6 5827-05-4 5834-96-8
5836-29-3 5840-95-9 5870-93-9 5895-18-1 5902-51-2
5902-79-4 5902-85-2 5902-95-4 5902-97-6 5903-10-6
5915-41-3 5954-14-3 5964-35-2 5969-94-8 5980-82-5
6012-84-6 6028-57-5 6073-72-9 6120-20-3 6190-65-4
6273-99-0 6303-21-5, Phosphinic acid 6365-83-9 6369-97-7
6373-07-5, biological studies 6379-37-9 6385-58-6 6386-63-6
6392-46-7 6420-47-9 6423-72-9 6440-58-0 6484-52-2, Nitric acid ammonium salt, biological studies 6550-86-3 6552-12-1
6565-70-4 6597-78-0 6616-80-4 6683-19-8 6734-80-1
6753-47-5 6798-76-1 6834-92-0 6915-15-7 6923-22-4
6988-21-2 6998-60-3, Rifamycin 7076-63-3 7097-60-1
7110-49-8D, nickel complexes 7122-04-5 7159-99-1 7166-19-0
7173-51-5 7206-15-7 7206-27-1 7212-44-4 7257-41-2

7281-04-1 7286-69-3 7286-84-2 7287-19-6 7287-36-7
7292-16-2 7313-54-4 7320-34-5 7345-69-9 7350-09-6
7359-55-9 7379-26-2 7379-27-3 7411-47-4 7421-93-4
7429-90-5, Aluminum, biological studies 7437-35-6 7439-89-6,
Iron, biological studies 7439-92-1, Lead, biological studies
7439-97-6, Mercury, biological studies 7439-98-7, Molybdenum,
biological studies 7440-02-0, Nickel, biological studies
7440-22-4, Silver, biological studies 7440-23-5, Sodium,
biological studies 7440-36-0, Antimony, biological studies
7440-38-2, Arsenic, biological studies 7440-42-8, Boron,
biological studies
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
(methods and compns. for increasing efficacy of biol. active
ingredients such as antitumor agents)

IT 10138-04-2 10213-78-2 10233-94-0 10248-55-2 10254-48-5
10257-54-2 10265-92-6 10279-57-9 10290-12-7 10294-66-3
10309-97-4 10311-84-9 10326-21-3 10326-24-6 10331-57-4
10361-16-7 10361-37-2, Barium chloride (BaCl2), biological studies
10377-60-3 10380-28-6 10389-50-1 10402-15-0 10402-16-1
10453-86-8 10486-00-7 10540-29-1 10545-99-0, Sulfur chloride
(SCl2) 10548-10-4 10552-74-6 10555-76-7 10588-01-9
10605-10-4 10605-11-5 10605-21-7 11006-34-1 11056-06-7,
Bleomycin 11084-85-8, Sodium hypochlorite phosphate
(Na13(ClO)(PO4)4) 11096-18-7, Cufraneb 11096-42-7 11113-80-7,
Polyoxin 11125-96-5 11126-29-7 11138-47-9 11138-66-2,
Xanthan gum 11141-17-6 12001-20-6 12002-03-8, C.I.
Pigment Green 21 12002-48-1 12002-53-8 12007-92-0,
Boron sodium oxide (B5NaO8) 12008-41-2, Boron sodium oxide
(B8Na2O13) 12018-01-8, Chromium oxide (CrO2) 12040-72-1
12057-74-8, Magnesium phosphide (Mg3P2) 12062-24-7 12068-06-3
12068-08-5 12068-09-6 12068-12-1 12068-15-4 12068-16-5
12071-83-9 12122-67-7 12124-97-9, Ammonium bromide ((NH4)Br)
12125-02-9, Ammonium chloride ((NH4)Cl), biological studies
12158-97-3, Copper oxide sulfate (Cu3O2(SO4)) 12168-20-6, Copper
iron hydroxide sulfate (CuFe(OH)2(SO4)) 12179-04-3 12219-26-0,
C.I. Acid Blue 182 12276-01-6 12280-03-4 12298-68-9, Potassium
iodide (K(I3)) 12328-56-2 12379-42-9 12379-51-0 12379-54-3
12379-66-7 12407-86-2 12427-38-2 12447-61-9 12616-49-8,
Plurafac C 17 12645-53-3 12680-48-7, Chromium sodium oxide
12701-72-3 12770-24-0, Toximul-P 12771-68-5 12789-03-6,
Chlordane 13010-20-3 13010-47-4 13067-93-1 13071-79-9
13114-87-9 13121-70-5 13171-21-6 13194-48-4 13302-00-6
13311-84-7 13331-52-7 13333-87-4 13347-42-7 13356-08-6
13358-11-7 13360-45-7 13387-91-2 13410-01-0 13426-91-0
13429-27-1 13445-49-3, Peroxydisulfuric acid ([(HO)S(O)2]2O2)
13446-48-5 13452-77-2 13455-24-8 13457-18-6 13463-41-7
13463-67-7, Titanium oxide (TiO2), biological studies 13464-33-0
13464-38-5 13464-42-1 13464-44-3 13477-36-6 13492-26-7
13560-99-1 13586-82-8 13593-03-8 13593-08-3 13598-36-2,
Phosphonic acid, biological studies 13684-44-1 13684-56-5
13684-63-4 13701-59-2 13707-65-8 13780-06-8 13824-96-9
13826-35-2 13840-33-0 13845-36-8 13863-41-7, Bromine chloride
(BrCl) 13864-38-5 13909-09-6 13932-13-3 13952-84-6,
2-Butanamine 13977-65-6 13978-85-3 14024-55-6 14025-15-1
14025-21-9 14047-23-5 14089-43-1 14099-38-8 14214-32-5
14215-52-2 14265-44-2, Phosphate, biological studies 14275-57-1
14332-21-9, Hypoiodous acid 14351-44-1 14354-56-4 14357-82-5
14437-17-3 14437-20-8 14455-29-9 14484-64-1 14491-59-9
14697-50-8 14701-21-4, biological studies 14807-96-6, Talc

(Mg3H2(SiO3)4), biological studies 14808-60-7, Quartz (SiO2), biological studies 14816-16-1 14816-18-3 14816-20-7 14979-39-6 15096-52-3, Cryolite (Na3(AlF6)) 15263-52-2 15263-53-3 15275-07-7 15299-99-7 15302-91-7 15310-01-7 15337-60-7 15339-36-3 15415-64-2 15537-82-3 15545-48-9 15595-24-1 15652-38-7 15662-33-6 15663-27-1 15733-22-9 15773-35-0 15905-32-5 15972-60-8 16013-44-8 16039-52-4 16079-88-2 16102-92-4 16227-10-4 16228-00-5 16423-68-0 16509-79-8 16655-82-6 16672-87-0 16676-96-3 16709-30-1 16725-53-4 16751-55-6 16752-77-5 16828-95-8 16871-71-9 16893-85-9 16919-19-0 16940-66-2 16949-65-8 16974-11-1 16974-12-2 17029-22-0 17040-19-6 17080-02-3 17109-49-8 17125-80-3 17210-55-8 17356-42-2 17367-56-5 17375-41-6 17439-94-0 17466-29-4 17496-08-1 17572-97-3 17606-31-4 17699-14-8 17702-57-7 17804-35-2 18128-16-0 18128-17-1 18130-44-4 18181-70-9 18249-20-2 18357-78-3 18378-89-7 18467-88-4

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(methods and compns. for increasing efficacy of biol. active ingredients such as antitumor agents)

IT 18472-87-2 18479-55-5 18530-56-8 18691-97-9 18748-91-9 18794-84-8 18854-01-8 18883-66-4 19044-88-3 19379-90-9 19398-13-1 19480-43-4 19622-08-3 19622-19-6 19651-91-3 19660-77-6 19691-80-6 19766-89-3 19937-59-8 20276-83-9 20290-99-7 20427-58-1, Zinc hydroxide (Zn(OH)2) 20427-59-2, Copper hydroxide (Cu(OH)2) 20543-04-8 20711-10-8 20762-60-1, Potassium azide (K(N3)) 20782-58-5 20830-81-3 20859-73-8, Aluminum phosphide (AlP) 20940-37-8 21087-64-9 21267-72-1 21351-39-3 21452-18-6 21540-35-2 21548-32-3 21564-17-0 21609-90-5 21645-51-2, Aluminum hydroxide (Al(OH)3), biological studies 21652-27-7 21689-84-9 21725-46-2 21832-25-7 21908-53-2, Mercury oxide (HgO) 21921-96-0 21923-23-9 22205-45-4, Copper sulfide (Cu2S) 22212-55-1 22212-56-2 22221-10-9 22221-12-1 22221-14-3 22224-92-6 22232-15-1 22232-20-8 22232-26-4 22232-28-6 22248-79-9 22259-30-9 22323-45-1 22330-14-9 22439-40-3 22569-74-0 22781-23-3 22894-47-9 22898-01-7 22936-75-0 22936-86-3 23031-36-9 23103-98-2 23121-99-5 23135-22-0 23184-66-9 23214-92-8 23319-66-6, biological studies 23422-53-9 23505-41-1 23526-02-5 23560-59-0 23564-05-8 23564-06-9 23710-76-1 23947-60-6 23950-58-5 23950-58-5D, metabolites 24017-47-8 24124-25-2 24151-93-7 24307-26-4 **24310-40-5** **24310-41-6** 24353-58-0 24353-61-5 24556-64-7 24556-65-8 24579-73-5 24691-76-7 24691-80-3 24927-67-1 24934-91-6 25013-16-5 25035-26-1 25059-78-3 25085-34-1 25086-29-7 25154-52-3 25155-30-0 25167-82-2 25167-83-3 25167-83-3D, alkylamine salt 25167-83-3D, coco-amine salt 25168-06-3 25168-15-4 25168-26-7 25171-63-5 25182-03-0 25254-50-6 25311-71-1 25316-56-7 25322-20-7 25322-68-3D, C10-C14 alkyl ethers, phosphates 25322-68-3D, alkyl ethers 25339-17-7, Isodecanol 25366-23-8 25402-06-6 25550-58-7 25567-55-9 25568-84-7 25606-41-1 25655-41-8 25671-46-9 25956-17-6 26002-80-2 26027-38-3 26062-79-3 26087-47-8 26129-32-8 26172-55-4 26248-24-8 26259-45-0 26264-05-1 26354-18-7 26389-78-6 26399-36-0 26419-73-8 26530-09-6 26530-20-1 26532-22-9 26532-23-0 26532-24-1 26532-25-2 26545-53-9 26617-87-8D, C10-18 alkyl derivs. 26617-87-8D, C12-15 alkyl derivs. 26617-87-8D, alkyl derivs. 26628-22-8, Sodium azide (Na(N3)) 26648-01-1 26761-40-0 26836-07-7 26856-61-1

26896-20-8, Neodecanoic acid 26952-20-5 27041-82-3 27041-84-5
27176-87-0 27177-77-1 27193-28-8 27193-86-8 27236-65-3
27252-87-5 27253-29-8 27304-13-8 27306-78-1 27323-41-7
27386-64-7 27458-93-1, Isooctadecanol 27519-02-4 27541-88-4
27554-26-3 27605-76-1 27636-20-0D, acetalized 27668-52-6
27923-56-4 27954-37-6 27987-00-4 28079-04-1 28086-13-7
28159-98-0 28217-97-2 28249-77-6 28300-74-5 28382-15-2
28401-39-0 28434-00-6 28434-01-7 28558-32-9 28559-00-4
28675-11-8 28730-17-8 28772-56-7 28801-69-6 28805-78-9
28837-97-0 28855-27-8 28956-64-1 29012-39-3D, derivs.
29061-61-8 29082-74-4 29091-05-2 29091-21-2 29173-31-7
29232-93-7 29385-43-1 29450-57-5 29457-72-5 29672-19-3
29804-22-6 29868-16-4 29871-13-4 29932-85-2 29973-13-5
30043-49-3 30043-55-1 30087-47-9 30136-13-1 30143-22-7
30284-78-7 30304-30-4 30507-70-1 30525-89-4, Paraformaldehyde
30551-20-3, Dodecadienal 30560-19-1 30622-37-8 30820-22-5
30864-28-9 30894-16-7
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methods and compns. for increasing efficacy of biol. active ingredients such as antitumor agents)

IT 53404-40-3 53404-43-6 53404-45-8 53404-46-9 53404-47-0
53404-49-2 53404-52-7 53404-53-8 53404-54-9 53404-55-0
53404-57-2 53404-58-3 53404-59-4 53404-67-4 53404-68-5
53404-69-6 53404-70-9 53404-71-0 53404-72-1 53404-77-6
53404-81-2 53404-82-3 53404-83-4 53404-84-5 53404-86-7
53404-87-8 53404-88-9 53404-89-0 53404-92-5 53404-93-6
53433-01-5 53433-02-6 53466-66-3 53466-87-8 53466-90-3
53466-93-6 53466-95-8 53466-98-1 53467-01-9 53494-70-5
53535-27-6 53535-32-3 53535-37-8 53537-62-5 53537-63-6
53637-60-8, Plurafac B 26 53663-71-1 53714-56-0 53780-34-0
53780-36-2 53819-72-0 53908-27-3 53910-25-1 53939-27-8
53939-28-9 53988-06-0 53988-93-5 54364-62-4 54453-03-1
54593-83-8 54774-45-7 54844-65-4 54864-61-8 55069-68-6
55072-57-6, Copper zinc hydroxide sulfate 55179-31-2 55195-26-1
55219-65-3 55256-33-2 55283-68-6 55285-14-8 55335-06-3
55406-53-6 55634-91-8 55635-13-7 55684-94-1 55701-05-8
55802-63-6, Zinc hydroxide sulfate 55807-46-0 55814-41-0
55861-78-4 55871-01-7 55871-02-8 55965-84-9 55965-87-2
56070-16-7 56073-07-5 56073-10-0 56141-00-5 56218-79-2
56219-04-6 56320-22-0, Arsenic sulfide (AsS2) 56425-91-3
56507-37-0 56573-85-4, Tin-San 56578-18-8 56634-95-8
56681-55-1 56683-54-6 56717-11-4 56750-76-6 56797-40-1
56855-08-4D, N-C12-14 alkyl, chloride 57018-04-9 57052-04-7
57063-29-3 57130-91-3 57213-69-1 57249-19-1 57369-32-1
57373-19-0 57373-20-3 57375-63-0 57455-37-5, C.I.
Pigment Blue 29 57646-30-7 57754-85-5 57837-19-1
57866-49-6 57966-95-7 57981-60-9 58001-44-8 58011-68-0
58175-59-0 58175-60-3 58594-45-9 58594-72-2 58594-74-4
58667-63-3 58810-48-3 58829-95-1 59010-86-5 59014-03-8
59026-08-3 59401-04-6 59644-67-6, Sterox NJ 59669-26-0
59915-53-6 60018-97-5 60037-58-3 60074-25-1 60168-88-9
60207-31-0 60207-90-1 60207-93-4 60238-56-4 60569-74-6,
Daxad 23 60742-37-2 60816-37-7 60825-27-6 60840-85-9
60864-33-7 61019-78-1 61167-10-0 61228-92-0 61432-55-1
61566-21-0 61614-62-8 61676-87-7 61827-83-6 61827-84-7
62031-70-3, Wingstay V 62046-37-1 62449-69-8 62476-59-9
62732-91-6 62850-32-2 62865-36-5 62924-70-3 63100-33-4,
Triton X 363 63284-71-9 63517-71-5 63517-72-6 63729-98-6
63744-60-5 63782-90-1 63798-77-6, Panasol AN 2 63837-33-2

63935-38-6 63992-41-6 64249-01-0 64359-80-4 64359-81-5
64491-92-5 64628-44-0 64700-56-7 64726-91-6 64902-72-3
65128-96-3 65271-80-9 65277-42-1 65666-57-1, Astrazon Yellow
65731-84-2 65733-18-8 65863-15-2, Alkanol XC 65907-30-4
65934-95-4 65954-19-0 66063-05-6 66159-95-3 66215-27-8
66227-09-6 66230-04-4 66246-88-6 66267-77-4 66332-96-5
66348-55-8 66441-11-0 66441-23-4 66841-24-5 66841-25-6
66952-49-6 67053-55-8, Toximul D 67129-08-2 67233-85-6
67306-00-7 67375-30-8 67446-07-5 67564-91-4 67674-67-3
67747-09-5 67923-62-0 67989-88-2 67992-60-3 68084-55-9
68085-85-8 68157-60-8 68214-43-7 68228-18-2 68228-19-3
68228-20-6 68240-09-5 68359-37-5 68505-69-1 68610-00-4
68694-11-1 68813-94-5
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methods and compns. for increasing efficacy of biol. active ingredients such as antitumor agents)

IT 68814-04-0, C.I. **Pigment** Yellow 115 68921-42-6
68957-70-0 69126-94-9D, derivs. 69254-40-6 69280-13-3,
Hostaphat MDAR-N 040 69309-47-3 69312-67-0 69335-91-7
69409-94-5 69462-12-0 69484-12-4 69484-13-5 69484-14-6
69516-34-3 69581-33-5 69632-93-5 69632-97-9 69632-98-0
69633-04-1 69653-69-6 69770-45-2 69806-34-4 69806-40-2
69806-50-4 69820-27-5 70024-53-2 70124-77-5 70193-21-4
70217-36-6 70393-85-0 70630-17-0 71283-80-2 71317-73-2
71526-07-3 71561-11-0 71626-11-4 71697-59-1 71751-41-2,
Avermectin B1 72146-51-1, Morwet IP 72178-02-0 72269-48-8
72348-92-6 72459-58-6 72490-01-8 72598-35-7 72850-64-7
72915-82-3 72963-72-5 73250-68-7 73394-27-1 73468-21-0,
Atplus 300F 73519-50-3 73886-28-9 73989-17-0, Avermectin
74051-80-2 74070-46-5 74222-97-2 74223-56-6 74223-64-6
74712-19-9 74738-17-3 74782-23-3 75497-92-6 75736-33-3
75747-77-2 76120-02-0 76397-81-4 76416-93-8, Tenneco 500-100
76578-12-6 76578-14-8 76608-88-3 76674-21-0 76738-62-0
76930-44-4, Po-san A 77182-82-2 77207-01-3 77227-69-1
77501-60-1 77501-63-4 77503-28-7 77503-29-8 77732-09-3
78110-38-0 78327-32-9 78357-48-9 78370-21-5 78403-23-3
78863-62-4 79241-46-6 79277-27-3 79277-67-1 79510-48-8
79538-32-2 79540-50-4 79622-59-6 79910-32-0 79983-71-4
80060-09-9 80625-77-0 81334-34-1 81335-37-7 81335-46-8
81335-47-9 81335-77-5 81412-43-3, Tridemorph 81510-83-0
81591-81-3 82010-74-0 82010-75-1 82010-77-3 82010-79-5
82010-82-0 82010-83-1 82027-59-6 82097-50-5 82211-24-3
82558-50-7 82560-54-1 82633-79-2 82657-04-3 82692-44-2
82810-23-9D, alkyl ethers 83055-99-6 83121-18-0 83130-01-2
83164-33-4 83318-76-7 83542-69-2 83542-80-7 83542-83-0
83601-83-6 83657-22-1 83657-24-3 83733-82-8 83869-01-6, TF 310 83982-06-3D, N-alkyl, sodium salt, complex with iodine
84082-88-2 84082-93-9 84332-86-5 84478-52-4 84496-56-0
85411-41-2, T-Mulz AO 2 85509-19-9 85785-20-2 86209-51-0
86479-06-3 86598-92-7 86763-47-5 86848-85-3 87130-20-9
87237-48-7 87310-56-3 87392-12-9 87547-04-4 87674-68-8
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94189-31-8, Stepantan A 94361-06-5 94593-91-6 95465-99-9
95480-33-4 95507-03-2 95977-29-0 96182-53-5 96491-05-3

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111988-49-9 111991-09-4 112226-61-6
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methods and compns. for increasing efficacy of biol. active ingredients such as antitumor agents)

L65 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:269996 HCAPLUS
DOCUMENT NUMBER: 140:303691
TITLE: Preparation and pharmaceutical compositions of novel pyrazolopyrimidines as cyclin dependent kinase inhibitors
INVENTOR(S): Guzi, Timothy J.; Paruch, Kamil; Dwyer, Michael P.; Doll, Ronald J.; Girijavallabhan, Viyyoor Moopil; Alvarez, Carmen S.; Chan, Tin-Yau; Knutson, Chad; Madison, Vincent; Fischmann, Thierry O.; Dillard, Lawrence W.; Tran, Vinh D.; He, Zhen Min; James, Ray Anthony; Park, Haengsoon
PATENT ASSIGNEE(S): Schering Corporation, USA; Pharmacopeia, Inc.
SOURCE: PCT Int. Appl., 91 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004026229	A2	20040401	WO 2003-US27491	20030903
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WO 2004026229	A3	20040617		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NI, NO, NZ, PG, PH, PL, PT, RO, RU, SC, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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JP 2006502184	T2	20060119	JP 2004-537708	200309 03
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ZA 2005001846	A	20050912	ZA 2005-1846	200503 03
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PRIORITY APPLN. INFO.:			US 2002-408029P P	200209 04
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			WO 2003-US27491 W	200309 03

OTHER SOURCE(S): MARPAT 140:303691

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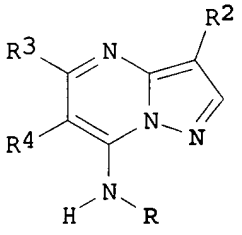

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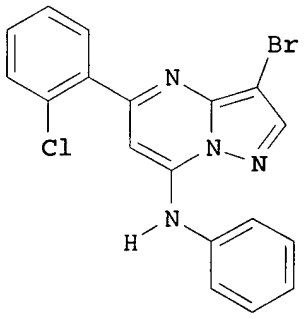
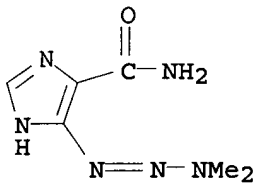


II

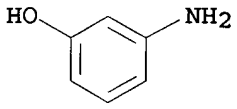
AB In its many embodiments, the present invention provides a novel class of pyrazolo[1,5-a]pyrimidine compds. I [R = (un)substituted aryl; R2 = halo, CN, (un)substituted alkyl, etc.; R3 = H, halo, (un)substituted-alkyl, -alkynyl, -aryl, etc.; R4 = H, halo or alkyl] as inhibitors of cyclin dependent kinases, methods of prepg. such compds., pharmaceutical compns. contg. one or more such compds., methods of prepg. pharmaceutical formulations comprising one or more such compds., and methods of treatment, prevention, inhibition, or amelioration of one or more diseases assocd. with the CDKs using such compds. or pharmaceutical compns. Thus, e.g., II was prepd. by substitution of 3-bromo-7-chloro-5-(2-chlorophenyl)-pyrazolo[1,5-a]pyrimidine (prepn. given) with aniline. I exhibit excellent CDK

inhibitory properties as demonstrated by II which possessed a IC50 value of 0.51 μM in kinase activity assays.

IT **4342-03-4**, Dacarbazine
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(claimed codrugs for treatment of conditions mediated by cyclin dependent kinases in the presence of prepd. pyrazolopyrimidines)
RN 4342-03-4 HCAPLUS
CN 1H-Imidazole-4-carboxamide, 5-(3,3-dimethyl-1-triazenyl)- (9CI) (CA INDEX NAME)



IT **591-27-5**, 3-Hydroxyaniline
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; prepn. of pyrazolopyrimidines as cyclin dependent kinase inhibitors)
RN 591-27-5 HCAPLUS
CN Phenol, 3-amino- (9CI) (CA INDEX NAME)



IC ICM A61K
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
IT Acute lymphocytic leukemia
Acute myeloid leukemia
Acute promyelocytic leukemia
Antitumor agents
Bladder, neoplasm
Chronic myeloid leukemia
Drug delivery systems
Drug interactions
Esophagus, neoplasm
Gallbladder, neoplasm
Hairy cell leukemia
Hodgkin's disease
Human
Kidney, neoplasm
Leukemia
Liver, neoplasm
Lung, neoplasm
Mammary gland, neoplasm
Melanoma
Myelodysplastic syndromes
Neuroglia, neoplasm
Ovary, neoplasm
Pancreas, neoplasm

Prostate gland, neoplasm
Skin, neoplasm
Stomach, neoplasm
Thyroid gland, neoplasm
(prepn. of pyrazolopyrimidines as cyclin dependent kinase inhibitors)

IT Skin, disease
(xeroderma **pigmentosum**; prepn. of pyrazolopyrimidines as cyclin dependent kinase inhibitors)

IT 50-07-7, Mitomycin-C 50-18-0, Cyclophosphamide 50-24-8, Prednisolone 50-44-2, 6-Mercaptopurine 50-76-0, Dactinomycin 50-91-9, Floxuridine 51-18-3, Triethylenemelamine 51-21-8, 5-Fluorouracil 51-75-2, Chlormethine 52-24-4, Triethylenethiophosphoramide 53-03-2, Prednisone 53-19-0, Mitotane 54-91-1, Pipobroman 55-98-1, Busulfan 56-53-1, Diethylstilbestrol 57-22-7, Vincristine 57-63-6, 17α-Ethinylestradiol 58-05-9, Leucovorin 58-18-4, Methyltestosterone 58-22-0, Testosterone 59-05-2, Methotrexate 66-75-1, Uracil mustard 68-96-2, Hydroxyprogesterone 71-58-9, Medroxyprogesterone acetate 76-43-7, Fluoxymesterone 83-43-2, Methylprednisolone 124-88-9 124-94-7, Triamcinolone 125-84-8, Aminoglutethimide 127-07-1, Hydroxyurea 147-94-4, Ara-C 148-82-3, Melphalan 154-42-7, 6-Thioguanine 154-93-8, Carmustine 305-03-3, Chlorambucil 521-12-0, Dromostanolone propionate 569-57-3, Chlorotrianisene 595-33-5, Megestrolacetate 645-05-6, Hexamethylmelamine 671-16-9, Procarbazine 865-21-4, Vinblastine 968-93-4, Testolactone 2998-57-4, Estramustine 3778-73-2, Ifosfamide **4342-03-4**, Dacarbazine 9015-68-3, L-Asparaginase 10540-29-1, Tamoxifen 11056-06-7, Bleomycin 13010-47-4, Lomustine 13311-84-7, Flutamide 14769-73-4, Levamisole 15663-27-1, Cisplatin 18378-89-7, Mithramycin 18883-66-4, Streptozocin 20830-81-3, Daunorubicin 23214-92-8, Doxorubicin 25316-40-9, Adriamycin 29767-20-2, Teniposide 33069-62-4, Taxol 33419-42-0, Etoposide 41575-94-4, Carboplatin 51264-14-3, Amsacrine 53643-48-4, Vindesine 53714-56-0, Leuprolide 53910-25-1, Pentostatin 56420-45-2, Epirubicin 58957-92-9, Idarubicin 61825-94-3, Oxaliplatin 65271-80-9, Mitoxantrone 65807-02-5, Goserelin 75607-67-9, Fludarabine phosphate 85622-93-1, Temozolomide 89778-26-7, Toremifene 95058-81-4, Gemcitabine 97682-44-5, Irinotecan 100286-90-6, CPT-11 112809-51-5, Letrozole 114977-28-5, Taxotere 120511-73-1, Anastrozole 123948-87-8, Topotecan 125317-39-7, Navelbine 154361-50-9, Capecitabine 183319-69-9, Tarceva 184475-35-2, Iressa 192185-68-5 193275-84-2, SCH 66336 195987-41-8 220127-57-1, Gleevec 253863-00-2, L778123
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(claimed codrugs for treatment of conditions mediated by cyclin dependent kinases in the presence of prepd. pyrazolopyrimidines)

IT 62-53-3, Aniline, reactions 78-96-6, 1-Amino-2-propanol 94-02-0, Ethyl benzoylacetate 100-46-9, Benzylamine, reactions 104-94-9, 4-Methoxyaniline 105-53-3, Diethyl malonate 107-10-8, 1-Propanamine, reactions 108-00-9, N,N-Dimethylethylenediamine 108-42-9, 3-Chloroaniline 108-91-8, Cyclohexylamine, reactions 109-01-3, N-Methylpiperazine 109-55-7, N,N-Dimethylpropylenediamine 109-85-3, 2-Aminoethyl methyl ether 111-42-2, N,N-Bis-2-hydroxyethylamine, reactions 115-69-5 121-47-1, 3-Aminobenzenesulfonic acid 121-57-3, 4-Aminobenzenesulfonic acid 141-78-6, Ethyl acetate, reactions 156-87-6, 3-Amino-1-propanol 504-24-5, 4-Aminopyridine 534-03-2 536-90-3, 3-Methoxyaniline **591-27-5**, 3-Hydroxyaniline

616-34-2, Methyl aminoacetate 933-88-0, 2-Methylbenzoyl chloride
1003-03-8, Aminocyclopentane 1484-84-0, 2-Piperidineethanol
1820-80-0, 3-Aminopyrazole 1877-77-6, 3-Aminobenzylalcohol
2026-48-4 2038-03-1, N-(2-Aminoethyl)morpholine 2524-67-6,
4-(N-Morpholino)-aniline 2719-27-9, Cyclohexanecarbonyl chloride
2905-60-4, 2,3-Dichlorobenzoyl chloride 3182-95-4 3433-37-2,
2-Piperidinemethanol 3535-37-3, 3,4-Dimethoxybenzoyl chloride
3731-51-9, 2-Aminomethylpyridine 3731-52-0, 3-Aminomethylpyridine
4276-09-9 5036-48-6, 1H-Imidazole-1-propanamine 5267-64-1
5271-67-0, Thiophene-2-carbonyl chloride 5292-21-7,
2-Cyclohexylacetic acid 5470-49-5, 4-Methylsulfonylaniline
5691-15-6, cis-1-Amino-2-hydroxymethylcyclohexane 5691-21-4,
trans-1-Amino-2-hydroxymethylcyclohexane 6168-72-5,
2-Aminopropan-1-ol 6575-24-2, (2,6-Dichlorophenyl)acetic acid
7065-46-5, 3,3-Dimethylbutanoyl chloride 7663-77-6 10314-99-5
10316-79-7 16617-46-2, 3-Amino-4-cyanopyrazole 21615-34-9,
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672325-06-3 672325-07-4 672325-08-5 672325-09-6 672325-10-9
672325-11-0 672325-12-1 672325-13-2 672325-24-5 672325-27-8
672325-38-1 673475-71-3 673475-72-4 674297-92-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; prepn. of pyrazolopyrimidines as cyclin dependent kinase inhibitors)

L65 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:203642 HCAPLUS
DOCUMENT NUMBER: 140:258598
TITLE: Diazonium compounds for **hair coloring** systems
INVENTOR(S): Adam, Jean-marie; Yousaf, Taher; Froehling, Beate; Eliu, Victor Paul
PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.
SOURCE: PCT Int. Appl., 147 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004019896	A1	20040311	WO 2003-EP9416	20030826

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,

EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

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CN 1678284	A	20051005	CN 2003-820608	200308 26
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JP 2006511721	T2	20060406	JP 2004-532111	200308 26
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US 2005251932	A1	20051117	US 2005-525300	200502 14
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PRIORITY APPLN. INFO.:			EP 2002-405753 A	200209 02
			<--	
			WO 2003-EP9416 W	200308 26

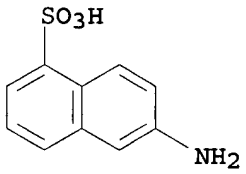
OTHER SOURCE(S): MARPAT 140:258598

AB A method of **coloring porous material**, esp. human **hair**, is described. The method comprises applying to the material being **colored**, in any desired order successively, or simultaneously, (a) at least one capped diazonium compd., and (b) at least one water-sol. coupling component, under conditions such that, initially, coupling does not take place, and then causing the capped diazonium compd. present on the material to react with the coupling component. For example, prepn. of a triazene **dye** was presented. 4-Chloro-2-amino-1-methylbenzene (43.4 g) was mixed with 81 g of 32% hydrochloric acid and cooled to 0°. Then, over the course of 1 h, 75 mL of 4 N aq. sodium nitrite soln. were added dropwise, with stirring, the temp. being maintained at 0-5°. The resulting soln. was then added dropwise, over the course of 15 min, to an aq. soln. of 30 g of sarcosine and 90 g of sodium carbonate in 250 mL of water at a temp. of 0-5°. The resulting brown suspension was filtered, the was recrystd. from ethanol and dried in air to afford 66.2 g of 3-methyl-1-(5-chloro-2-methylphenyl)-3-(carboxymethyl)triazene powder (yield: 91%). A strand of bleached human **hair** was immersed, for 30 min at room temp., in an aq. soln. contg. 0.2 M triazene and 0.2 M coupling component, which

has been adjusted to pH 10.0 using sodium carbonate, ammonia or NaOH. The strand was removed, excess soln. was wiped off and the strand was immersed for 5 min in a pH 3 buffer soln. contg. 4% sodium citrate and 2% citric acid. The strand was then thoroughly rinsed using water and, where appropriate, a shampoo soln. and was dried. **Hair** was **colored** with outstanding fastness properties, esp. fastness to washing properties.

IT **81-05-0 86-45-3 87-02-5 88-63-1**
90-20-0 90-40-4 90-51-7 99-11-6
108-46-3, 1,3-Benzenediol, biological studies
119-79-9 479-27-6, 1,8-Naphthalenediamine
591-27-5 6362-18-1 16867-03-1
31643-63-7 457629-66-2
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(coupling agent; **hair coloring** system comprising diazonium **dye** and coupling agent)

RN 81-05-0 HCAPLUS
CN 1-Naphthalenesulfonic acid, 6-amino- (8CI, 9CI) (CA INDEX NAME)



RN 86-45-3 HCAPLUS
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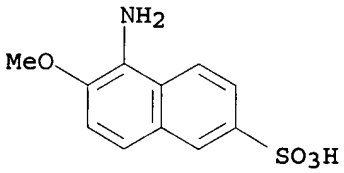
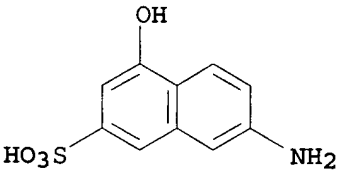
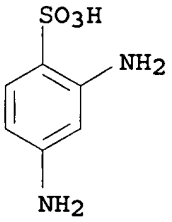


RN 87-02-5 HCAPLUS
CN 2-Naphthalenesulfonic acid, 7-amino-4-hydroxy- (8CI, 9CI) (CA INDEX NAME)



RN 88-63-1 HCAPLUS
CN Benzenesulfonic acid, 2,4-diamino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 90-20-0 HCAPLUS
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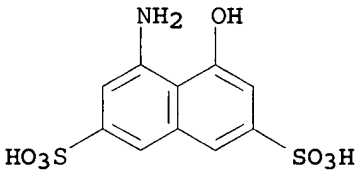
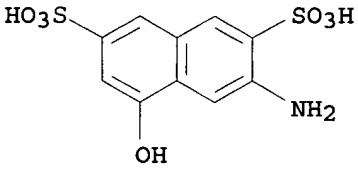
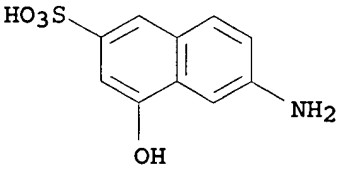


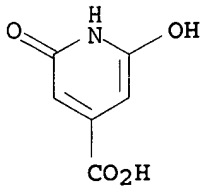
RN 90-40-4 HCAPLUS
CN 2,7-Naphthalenedisulfonic acid, 3-amino-5-hydroxy- (7CI, 8CI, 9CI) (CA INDEX NAME)



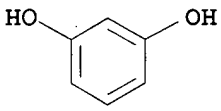
RN 90-51-7 HCAPLUS
CN 2-Naphthalenesulfonic acid, 6-amino-4-hydroxy- (8CI, 9CI) (CA INDEX NAME)



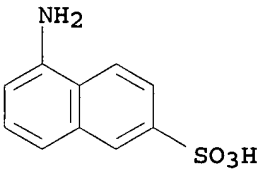
RN 99-11-6 HCAPLUS
CN 4-Pyridinecarboxylic acid, 1,2-dihydro-6-hydroxy-2-oxo- (9CI) (CA INDEX NAME)



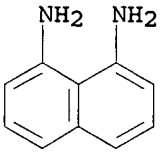
RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



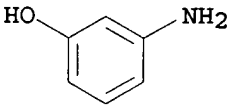
RN 119-79-9 HCAPLUS
CN 2-Naphthalenesulfonic acid, 5-amino- (8CI, 9CI) (CA INDEX NAME)



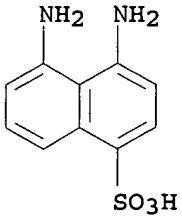
RN 479-27-6 HCAPLUS
CN 1,8-Naphthalenediamine (7CI, 8CI, 9CI) (CA INDEX NAME)



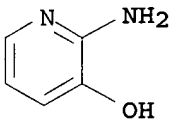
RN 591-27-5 HCAPLUS
CN Phenol, 3-amino- (9CI) (CA INDEX NAME)



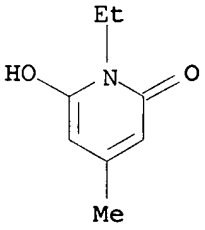
RN 6362-18-1 HCAPLUS
CN 1-Naphthalenesulfonic acid, 4,5-diamino- (8CI, 9CI) (CA INDEX NAME)



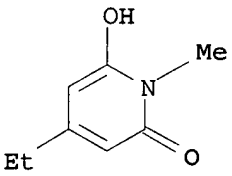
RN 16867-03-1 HCAPLUS
CN 3-Pyridinol, 2-amino- (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 31643-63-7 HCAPLUS
CN 2(1H)-Pyridinone, 1-ethyl-6-hydroxy-4-methyl- (9CI) (CA INDEX NAME)



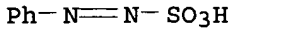
RN 457629-66-2 HCAPLUS
CN 2(1H)-Pyridinone, 4-ethyl-6-hydroxy-1-methyl- (9CI) (CA INDEX NAME)



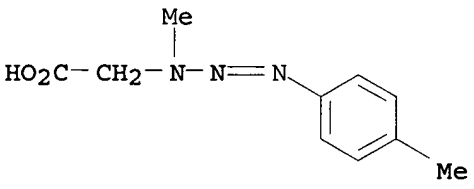
IT **30221-20-6P 51955-67-0P 67599-13-7P**
457629-58-2P 457629-59-3P 457629-60-6P
457629-65-1P 667878-10-6P 667878-12-8P
667878-14-0P 667878-16-2P 667878-17-3P
667878-19-5P 667878-20-8P 667878-22-0P
667878-24-2P 667878-25-3P 667878-27-5P
667878-29-7P 667878-31-1P 667878-34-4P
667878-36-6P 667878-38-8P 667878-40-2P
667878-41-3P 667878-42-4P 667878-44-6P
667878-45-7P 667878-47-9P 667878-49-1P
667878-51-5P 667878-53-7P 667878-54-8P
667878-56-0P 667878-58-2P 667878-60-6P
667878-63-9P

RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(**hair coloring** system comprising diazonium **dye** and coupling agent)

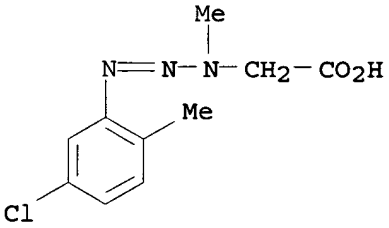
RN 30221-20-6 HCAPLUS
CN Diazenesulfonic acid, phenyl- (9CI) (CA INDEX NAME)



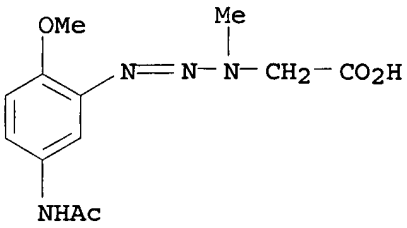
RN 51955-67-0 HCAPLUS
CN Acetic acid, [1-methyl-3-(4-methylphenyl)-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



RN 67599-13-7 HCAPLUS
CN Acetic acid, [3-(5-chloro-2-methylphenyl)-1-methyl-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)

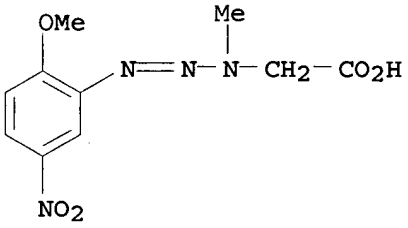


RN 457629-58-2 HCAPLUS
CN Acetic acid, [3-[5-(acetylamino)-2-methoxyphenyl]-1-methyl-2-triazenyl]-, monosodium salt (9CI) (CA INDEX NAME)



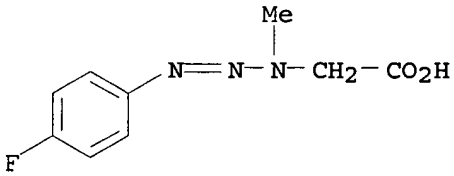
● Na

RN 457629-59-3 HCAPLUS
CN Acetic acid, [3-(2-methoxy-5-nitrophenyl)-1-methyl-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



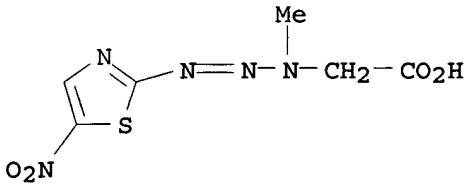
● Na

RN 457629-60-6 HCAPLUS
CN Acetic acid, [3-(4-fluorophenyl)-1-methyl-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



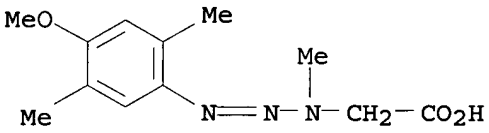
● Na

RN 457629-65-1 HCAPLUS
CN Acetic acid, [1-methyl-3-(5-nitro-2-thiazolyl)-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



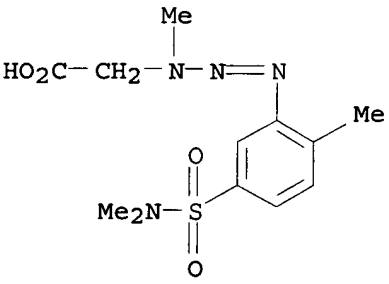
● Na

RN 667878-10-6 HCAPLUS
CN Acetic acid, [3-(4-methoxy-2,5-dimethylphenyl)-1-methyl-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



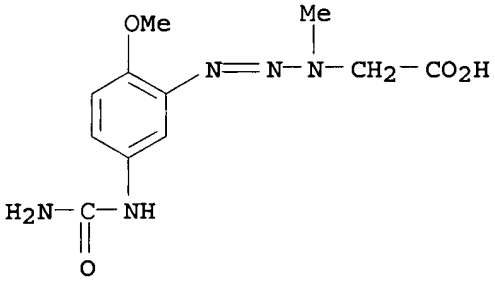
● Na

RN 667878-12-8 HCAPLUS
CN Acetic acid, [3-[5-[(dimethylamino)sulfonyl]-2-methylphenyl]-1-methyl-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



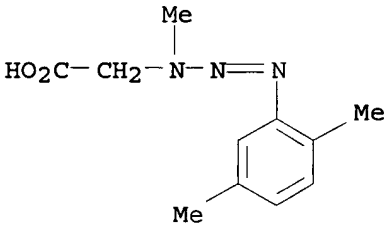
● Na

RN 667878-14-0 HCAPLUS
CN Acetic acid, [3-[5-[(aminocarbonyl)amino]-2-methoxyphenyl]-1-methyl-2-triazenyl]-, monosodium salt (9CI) (CA INDEX NAME)



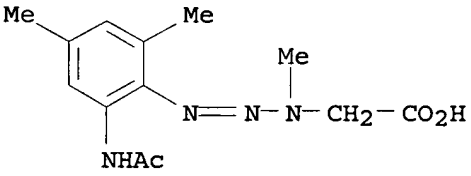
● Na

RN 667878-16-2 HCAPLUS
CN Acetic acid, [3-(2,5-dimethylphenyl)-1-methyl-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



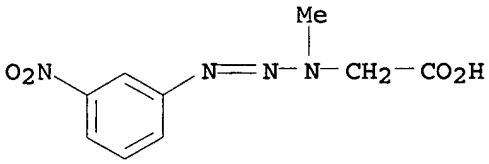
● Na

RN 667878-17-3 HCAPLUS
CN Acetic acid, [3-[2-(acetylamino)-4,6-dimethylphenyl]-1-methyl-2-triazenyl]-, monosodium salt (9CI) (CA INDEX NAME)



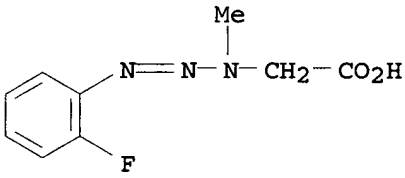
● Na

RN 667878-19-5 HCAPLUS
CN Acetic acid, [1-methyl-3-(3-nitrophenyl)-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



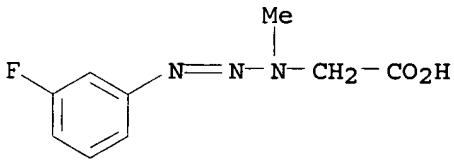
● Na

RN 667878-20-8 HCAPLUS
CN Acetic acid, [3-(2-fluorophenyl)-1-methyl-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



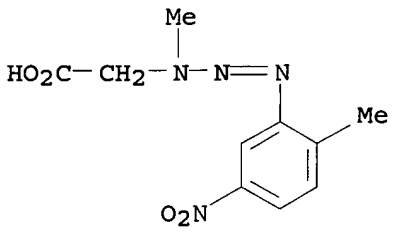
● Na

RN 667878-22-0 HCAPLUS
CN Acetic acid, [3-(3-fluorophenyl)-1-methyl-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



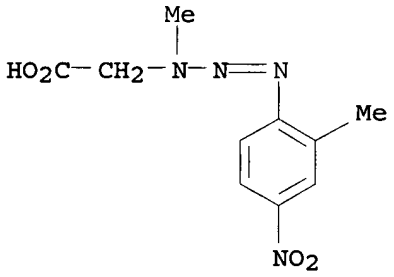
● Na

RN 667878-24-2 HCAPLUS
CN Acetic acid, [1-methyl-3-(2-methyl-5-nitrophenyl)-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



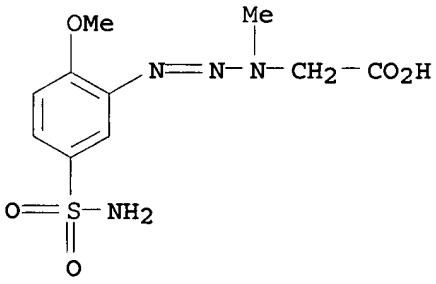
● Na

RN 667878-25-3 HCAPLUS
CN Acetic acid, [1-methyl-3-(2-methyl-4-nitrophenyl)-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



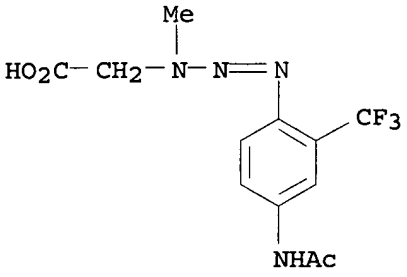
● Na

RN 667878-27-5 HCAPLUS
CN Acetic acid, [3-[5-(aminosulfonyl)-2-methoxyphenyl]-1-methyl-2-triazenyl]-, monosodium salt (9CI) (CA INDEX NAME)



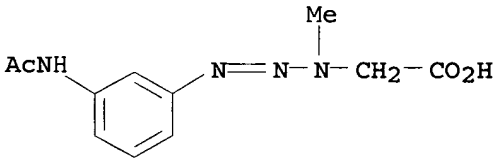
● Na

RN 667878-29-7 HCAPLUS
CN Acetic acid, [3-[4-(acetylamino)-2-(trifluoromethyl)phenyl]-1-methyl-2-triazenyl]-, monosodium salt (9CI) (CA INDEX NAME)



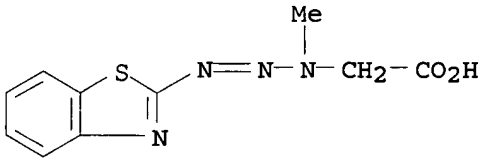
● Na

RN 667878-31-1 HCAPLUS
CN Acetic acid, [3-[3-(acetylamino)phenyl]-1-methyl-2-triazenyl]-, monosodium salt (9CI) (CA INDEX NAME)



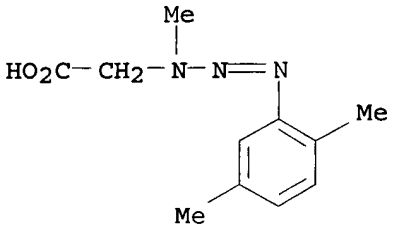
● Na

RN 667878-34-4 HCAPLUS
CN Acetic acid, [3-(2-benzothiazolyl)-1-methyl-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)

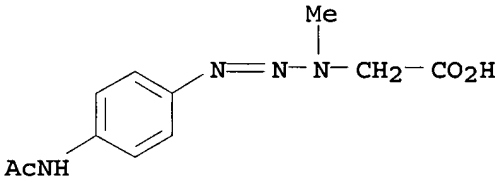


● Na

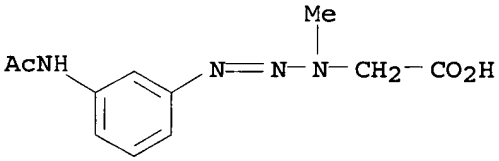
RN 667878-36-6 HCAPLUS
CN Acetic acid, [3-(2,5-dimethylphenyl)-1-methyl-2-triazenyl]- (9CI) (CA INDEX NAME)



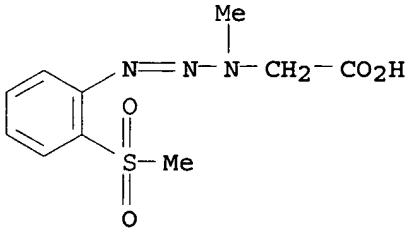
RN 667878-38-8 HCAPLUS
CN Acetic acid, [3-[4-(acetylamino)phenyl]-1-methyl-2-triazenyl]- (9CI) (CA INDEX NAME)



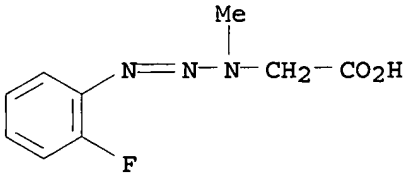
RN 667878-40-2 HCAPLUS
CN Acetic acid, [3-[3-(acetylamino)phenyl]-1-methyl-2-triazenyl]- (9CI) (CA INDEX NAME)



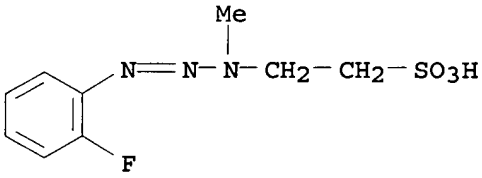
RN 667878-41-3 HCAPLUS
CN Acetic acid, [1-methyl-3-[2-(methylsulfonyl)phenyl]-2-triazenyl]- (9CI) (CA INDEX NAME)



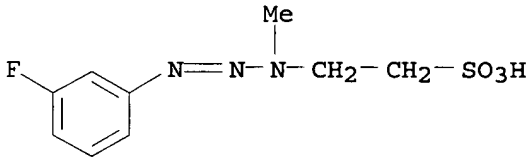
RN 667878-42-4 HCAPLUS
CN Acetic acid, [3-(2-fluorophenyl)-1-methyl-2-triazenyl]- (9CI) (CA INDEX NAME)



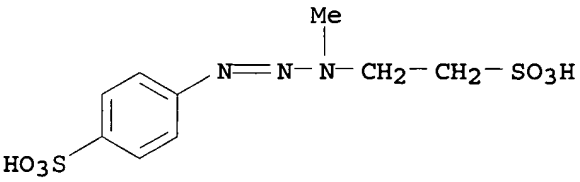
RN 667878-44-6 HCAPLUS
CN Ethanesulfonic acid, 2-[3-(2-fluorophenyl)-1-methyl-2-triazenyl]-
(9CI) (CA INDEX NAME)



RN 667878-45-7 HCAPLUS
CN Ethanesulfonic acid, 2-[3-(3-fluorophenyl)-1-methyl-2-triazenyl]-
(9CI) (CA INDEX NAME)

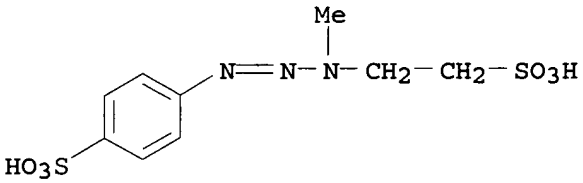


RN 667878-47-9 HCAPLUS
CN Benzenesulfonic acid, 4-[3-methyl-3-(2-sulfoethyl)-1-triazenyl]-,
disodium salt (9CI) (CA INDEX NAME)

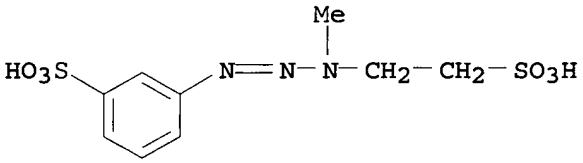


●2 Na

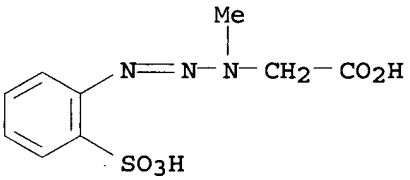
RN 667878-49-1 HCAPLUS
CN Benzenesulfonic acid, 4-[3-methyl-3-(2-sulfoethyl)-1-triazenyl]-
(9CI) (CA INDEX NAME)



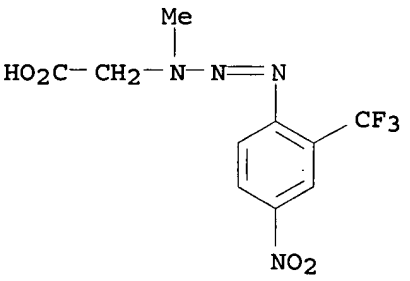
RN 667878-51-5 HCAPLUS
CN Benzenesulfonic acid, 3-[3-methyl-3-(2-sulfoethyl)-1-triazenyl]- (9CI) (CA INDEX NAME)



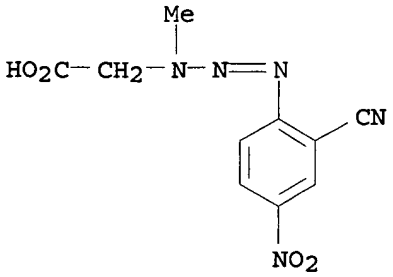
RN 667878-53-7 HCAPLUS
CN Acetic acid, [1-methyl-3-(2-sulfophenyl)-2-triazenyl]- (9CI) (CA INDEX NAME)



RN 667878-54-8 HCAPLUS
CN Acetic acid, [1-methyl-3-[4-nitro-2-(trifluoromethyl)phenyl]-2-triazenyl]- (9CI) (CA INDEX NAME)



RN 667878-56-0 HCAPLUS
CN Acetic acid, [3-(2-cyano-4-nitrophenyl)-1-methyl-2-triazenyl]- (9CI) (CA INDEX NAME)



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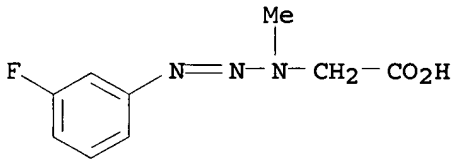
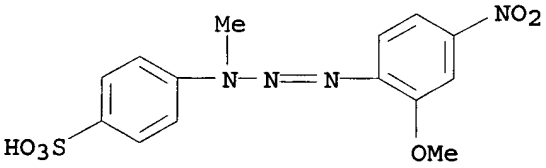
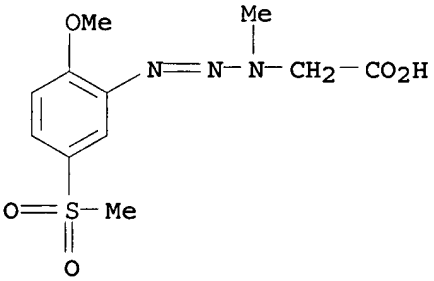
CN Acetic acid, [3-(3-fluorophenyl)-1-methyl-2-triazenyl]- (9CI) (CA INDEX NAME)



RN 667878-60-6 HCAPLUS
CN Benzenesulfonic acid, 4-[3-(2-methoxy-4-nitrophenyl)-1-methyl-2-triazenyl]- (9CI) (CA INDEX NAME)



RN 667878-63-9 HCAPLUS
CN Acetic acid, [3-[2-methoxy-5-(methylsulfonyl)phenyl]-1-methyl-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



● Na

IC ICM A61K007-13
ICS C09B067-00; C07C245-24
CC 62-3 (Essential Oils and Cosmetics)
Section cross-reference(s): 25
ST diazonium **dye** prepn coupling agent **hair coloring**
IT **Dyes**
(acid, combination with; **hair coloring** system comprising diazonium **dye** and coupling agent)
IT Diazonium compounds
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(arene; **hair coloring** system comprising diazonium **dye** and coupling agent)
IT **Dyes**
(cationic, combination with; **hair coloring** system comprising diazonium **dye** and coupling agent)
IT **Dyes**
(direct, combination with; **hair coloring** system comprising diazonium **dye** and coupling agent)
IT **Hair** preparations
(**dyes**, oxidative, combination with; **hair coloring** system comprising diazonium **dye** and coupling agent)
IT **Hair** preparations
(**dyes**; **hair coloring** system comprising diazonium **dye** and coupling agent)
IT Antioxidants
Human
UV stabilizers
(**hair coloring** system comprising diazonium **dye** and coupling agent)
IT Diazonium compounds
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(**hair coloring** system comprising diazonium **dye** and coupling agent)
IT 633-96-5, Orange No. 205
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(Orange No. 205; **hair coloring** system comprising diazonium **dye** and coupling agent)
IT **81-05-0 86-45-3 87-02-5 88-63-1**
90-20-0 90-40-4 90-51-7 99-11-6
108-46-3, 1,3-Benzenediol, biological studies
119-79-9 479-27-6, 1,8-Naphthalenediamine
591-27-5 6362-18-1 16867-03-1
31643-63-7 457629-66-2
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(coupling agent; **hair coloring** system comprising diazonium **dye** and coupling agent)
IT 1064-48-8, Japan Black 401 3177-22-8 4430-18-6, Japan Violet 401
7722-84-1, Hydrogen peroxide, biological studies 12270-25-6, Basic Red 51 61901-61-9, C.I. Basic Orange 31 359762-03-1
412015-79-3
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(**hair coloring** system comprising diazonium **dye** and coupling agent)
IT **30221-20-6P 51955-67-0P 67599-13-7P**
457629-58-2P 457629-59-3P 457629-60-6P
457629-65-1P 667878-10-6P 667878-12-8P

667878-14-0P 667878-16-2P 667878-17-3P
667878-19-5P 667878-20-8P 667878-22-0P
667878-24-2P 667878-25-3P 667878-27-5P
667878-29-7P 667878-31-1P 667878-34-4P
667878-36-6P 667878-38-8P 667878-40-2P
667878-41-3P 667878-42-4P 667878-44-6P
667878-45-7P 667878-47-9P 667878-49-1P
667878-51-5P 667878-53-7P 667878-54-8P
667878-56-0P 667878-58-2P 667878-60-6P
667878-63-9P
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(**hair coloring** system comprising diazonium **dye** and coupling agent)

IT 95-79-4 107-97-1, Sarcosine
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of triazenes for **hair coloring** system)

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L65 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:695738 HCAPLUS
DOCUMENT NUMBER: 137:221759
TITLE: Method of **coloring** human **hair** with compositions containing diazonium compounds
INVENTOR(S): Adam, Jean-Marie; Yousaf, Taher; Froehling, Beate
PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.
SOURCE: PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002069920	A1	20020912	WO 2002-EP2146	20020228
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W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1365732	A1	20031203	EP 2002-722158	20020228
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BR 2002007949	A	20040727	BR 2002-7949	200202 28
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JP 2004522787	T2	20040729	JP 2002-569098	200202 28
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NZ 527388	A	20050624	NZ 2002-527388	200202 28
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CN 1633275	A	20050629	CN 2002-806207	200202 28
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ZA 2003005754	A	20040713	ZA 2003-5754	200307 25
			<--	
US 2004083560	A1	20040506	US 2003-469619	200309 03
			<--	
US 7041143	B2	20060509		
PRIORITY APPLN. INFO.:			EP 2001-810240 A	200103 08
			<--	
			WO 2002-EP2146 W	200202 28
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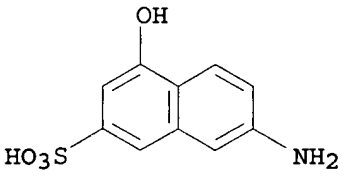
OTHER SOURCE(S): MARPAT 137:221759

AB A method of **coloring porous material**, esp. human **hair**, comprises applying to the material being **colored**, in any desired order successively, or simultaneously, a capped diazonium compd. and a water-sol. coupling component under conditions such that, initially, coupling does not take place, and then causing the capped diazonium compd. present on the material to react with the coupling component. Thus, a bleached human **hair** is **colored** with a mixt. of equal parts by wt. 5 g in each case of 6% H2O2 soln. and of the following compn. B. The compn. contained cetylstearyl alc. 11.00, Oleth-5 5.0, oleic acid 2.5, stearic acid monoethanolamide 2.5, coconut fatty acid monoethanolamide 2.5, sodium lauryl sulfate 1.7 1,2-propanediol 1.0, ammonium chloride 0.5, tetra-sodium EDTA 0.2, perfume 0.4, wheat protein hydrolyzate 0.2, silica 0.1, a triazene 9.32, 1,8-naphthalenediamine coupler 11.52, and water to 100%.

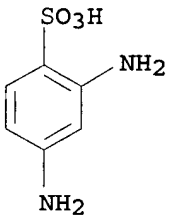
IT **87-02-5 88-63-1 90-20-0 90-40-4**
99-11-6 108-46-3, 1,3-Benzenediol, biological studies **119-79-9 479-27-6**, 1,8-Naphthalenediamine **591-27-5 16867-03-1**
22667-68-1 31643-63-7 33067-78-6
51955-66-9 51955-68-1 57103-28-3
67599-15-9 457629-60-6 457629-61-7
457629-62-8 457629-63-9 457629-64-0
457629-65-1 457629-66-2 457629-67-3
457629-69-5 457629-70-8 457629-71-9
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)

(method of **coloring** human **hair** with compns. contg. diazonium compds.)

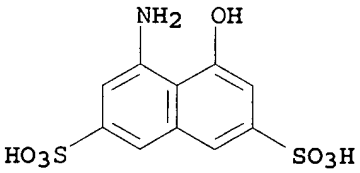
RN 87-02-5 HCAPLUS
CN 2-Naphthalenesulfonic acid, 7-amino-4-hydroxy- (8CI, 9CI) (CA INDEX NAME)



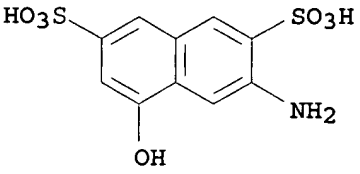
RN 88-63-1 HCAPLUS
CN Benzenesulfonic acid, 2,4-diamino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



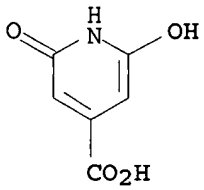
RN 90-20-0 HCAPLUS
CN 2,7-Naphthalenedisulfonic acid, 4-amino-5-hydroxy- (8CI, 9CI) (CA INDEX NAME)



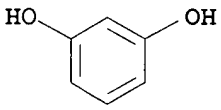
RN 90-40-4 HCAPLUS
CN 2,7-Naphthalenedisulfonic acid, 3-amino-5-hydroxy- (7CI, 8CI, 9CI) (CA INDEX NAME)



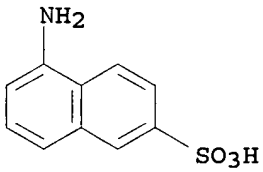
RN 99-11-6 HCAPLUS
CN 4-Pyridinecarboxylic acid, 1,2-dihydro-6-hydroxy-2-oxo- (9CI) (CA INDEX NAME)



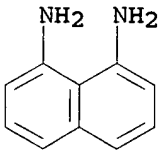
RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



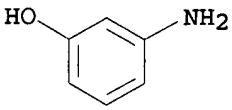
RN 119-79-9 HCAPLUS
CN 2-Naphthalenesulfonic acid, 5-amino- (8CI, 9CI) (CA INDEX NAME)



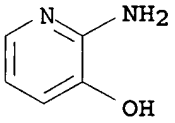
RN 479-27-6 HCAPLUS
CN 1,8-Naphthalenediamine (7CI, 8CI, 9CI) (CA INDEX NAME)



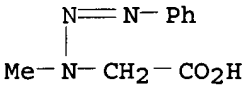
RN 591-27-5 HCAPLUS
CN Phenol, 3-amino- (9CI) (CA INDEX NAME)



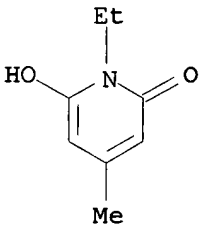
RN 16867-03-1 HCAPLUS
CN 3-Pyridinol, 2-amino- (6CI, 8CI, 9CI) (CA INDEX NAME)



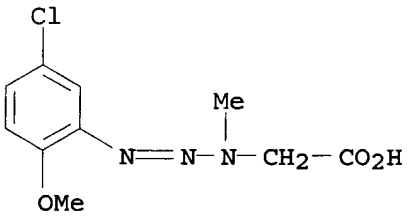
RN 22667-68-1 HCAPLUS
CN Acetic acid, (1-methyl-3-phenyl-2-triazenyl)- (9CI) (CA INDEX NAME)



RN 31643-63-7 HCAPLUS
CN 2(1H)-Pyridinone, 1-ethyl-6-hydroxy-4-methyl- (9CI) (CA INDEX NAME)

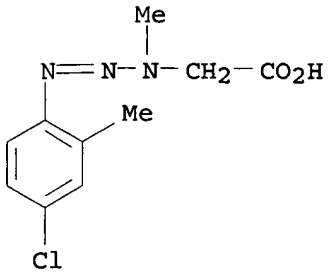


RN 33067-78-6 HCAPLUS
CN Acetic acid, [3-(5-chloro-2-methoxyphenyl)-1-methyl-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



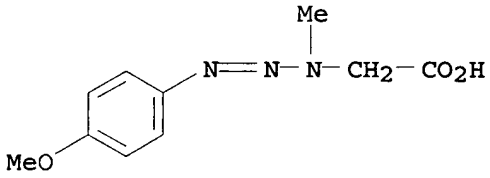
● Na

RN 51955-66-9 HCAPLUS
CN Acetic acid, [3-(4-chloro-2-methylphenyl)-1-methyl-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



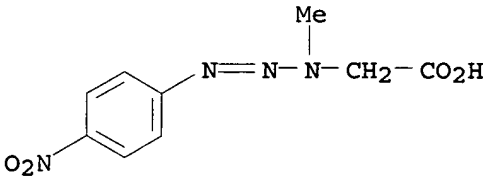
● Na

RN 51955-68-1 HCAPLUS
CN Acetic acid, [3-(4-methoxyphenyl)-1-methyl-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)

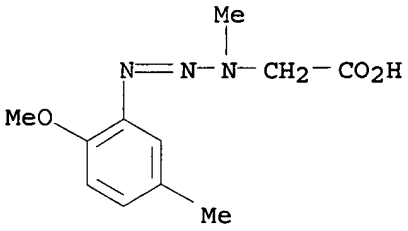


● Na

RN 57103-28-3 HCAPLUS
CN Acetic acid, [1-methyl-3-(4-nitrophenyl)-2-triazenyl]- (9CI) (CA INDEX NAME)

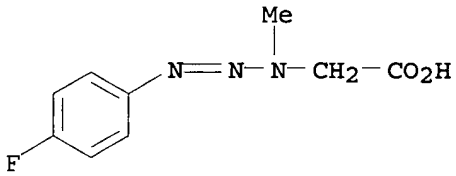


RN 67599-15-9 HCAPLUS
CN Acetic acid, [3-(2-methoxy-5-methylphenyl)-1-methyl-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



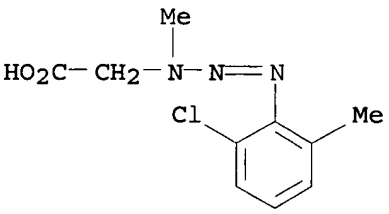
● Na

RN 457629-60-6 HCAPLUS
CN Acetic acid, [3-(4-fluorophenyl)-1-methyl-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



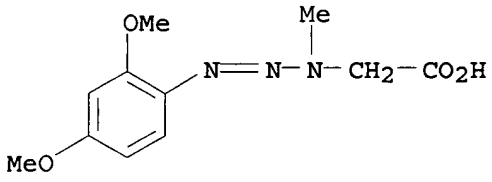
● Na

RN 457629-61-7 HCAPLUS
CN Acetic acid, [3-(2-chloro-6-methylphenyl)-1-methyl-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



● Na

RN 457629-62-8 HCAPLUS
CN Acetic acid, [3-(2,4-dimethoxyphenyl)-1-methyl-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



● Na

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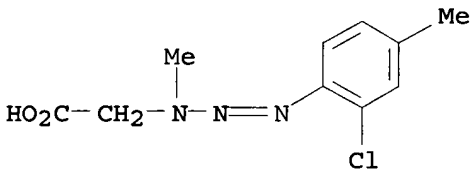
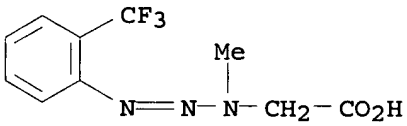


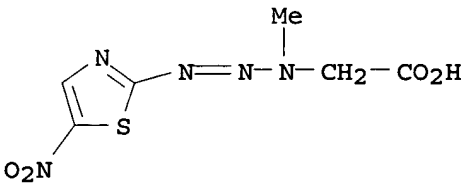
● Na

RN 457629-64-0 HCAPLUS
CN Acetic acid, [1-methyl-3-[2-(trifluoromethyl)phenyl]-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



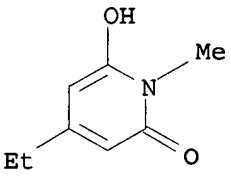
● Na

RN 457629-65-1 HCAPLUS
CN Acetic acid, [1-methyl-3-(5-nitro-2-thiazolyl)-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)

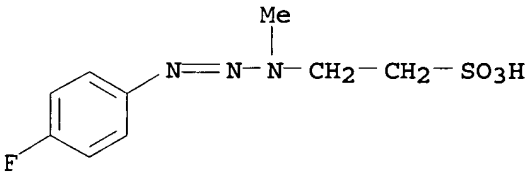


● Na

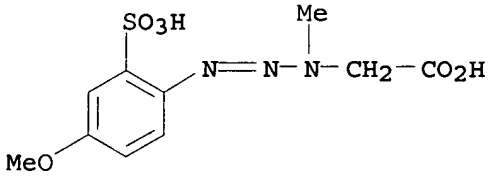
RN 457629-66-2 HCAPLUS
CN 2(1H)-Pyridinone, 4-ethyl-6-hydroxy-1-methyl- (9CI) (CA INDEX NAME)



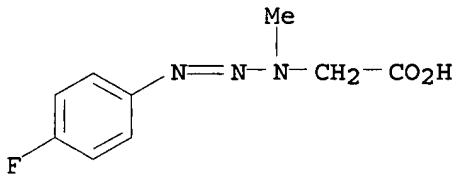
RN 457629-67-3 HCAPLUS
CN Ethanesulfonic acid, 2-[3-(4-fluorophenyl)-1-methyl-2-triazenyl]- (9CI) (CA INDEX NAME)



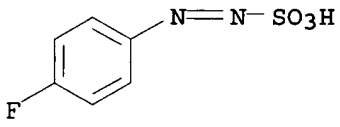
RN 457629-69-5 HCAPLUS
CN Acetic acid, [3-(4-methoxy-2-sulfophenyl)-1-methyl-2-triazenyl]- (9CI) (CA INDEX NAME)



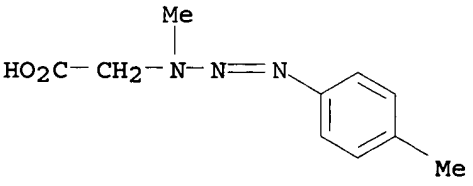
RN 457629-70-8 HCAPLUS
CN Acetic acid, [3-(4-fluorophenyl)-1-methyl-2-triazenyl]- (9CI) (CA INDEX NAME)



RN 457629-71-9 HCAPLUS
CN Diazenesulfonic acid, (4-fluorophenyl)- (9CI) (CA INDEX NAME)

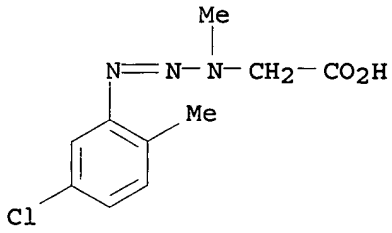


IT **51955-67-0P 67599-13-7P 457629-58-2P**
457629-59-3P
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(method of **coloring** human **hair** with compns. contg. diazonium compds.)
RN 51955-67-0 HCAPLUS
CN Acetic acid, [1-methyl-3-(4-methylphenyl)-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



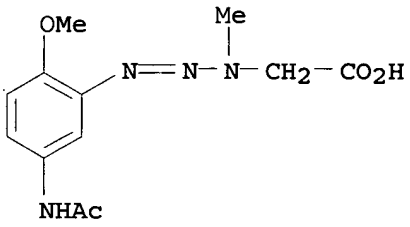
● Na

RN 67599-13-7 HCAPLUS
CN Acetic acid, [3-(5-chloro-2-methylphenyl)-1-methyl-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



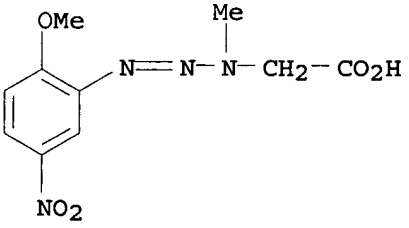
● Na

RN 457629-58-2 HCAPLUS
CN Acetic acid, [3-[5-(acetylamino)-2-methoxyphenyl]-1-methyl-2-triazenyl]-, monosodium salt (9CI) (CA INDEX NAME)



● Na

RN 457629-59-3 HCAPLUS
CN Acetic acid, [3-(2-methoxy-5-nitrophenyl)-1-methyl-2-triazenyl]-, sodium salt (9CI) (CA INDEX NAME)



● Na

IC ICM A61K007-13
ICS C09B067-00; C07C245-24
CC 62-3 (Essential Oils and Cosmetics)
Section cross-reference(s): 25
ST **hair coloring** diazonium compd prepn
IT **Hair** preparations
(**dyes**; method of **coloring** human **hair**

with compns. contg. diazonium compds.)
IT **Hair**
Human
(method of **coloring** human **hair** with compns. contg. diazonium compds.)
IT Diazonium compounds
Quaternary ammonium compounds, biological studies
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(method of **coloring** human **hair** with compns. contg. diazonium compds.)
IT **84-89-9 87-02-5 88-63-1 90-20-0 90-40-4 99-11-6 108-46-3**, 1,3-Benzenediol, biological studies **119-79-9 479-27-6**, 1,8-Naphthalenediamine **591-27-5 16867-03-1 22667-68-1 31643-63-7 33067-78-6 51955-66-9 51955-68-1 57103-28-3 67599-15-9** 74474-94-5 **457629-60-6 457629-61-7 457629-62-8 457629-63-9 457629-64-0 457629-65-1 457629-66-2 457629-67-3** 457629-68-4 **457629-69-5 457629-70-8 457629-71-9**
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(method of **coloring** human **hair** with compns. contg. diazonium compds.)
IT **51955-67-0P 67599-13-7P 457629-58-2P 457629-59-3P**
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(method of **coloring** human **hair** with compns. contg. diazonium compds.)
IT 95-79-4 107-97-1, Sarcosine
RL: RCT (Reactant); RACT (Reactant or reagent)
(method of **coloring** human **hair** with compns. contg. diazonium compds.)
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

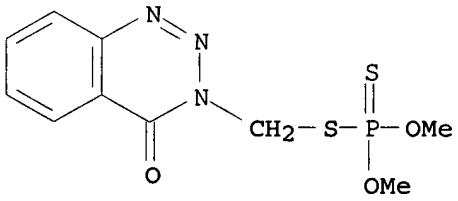
=> => d l66 ibib abs hitstr hitind 1-11

L66 ANSWER 1 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:749877 HCAPLUS
DOCUMENT NUMBER: 126:43857
TITLE: Prediction of rodent carcinogenicity bioassays from molecular structure using inductive logic programming
AUTHOR(S): King, Ross D.; Srinivasan, Ashwin
CORPORATE SOURCE: Biomolecular Modelling Laboratory, University Oxford, London, WC2A 3PX, UK
SOURCE: Environmental Health Perspectives Supplements (**1996**), 104(5), 1031-1040
CODEN: EHPSEO; ISSN: 1078-0475
PUBLISHER: National Institute of Environmental Health Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The machine learning program Progol was applied to the problem of forming the structure-activity relation (SAR) for a set of compds.

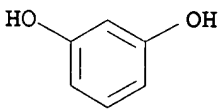
tested for carcinogenicity in rodent bioassays by the U.S. National Toxicol. Program (NTP). Progol is the first inductive logic programming (ILP) algorithm to use a fully relational method for describing chem. structure in SARs, based on using atoms and their bond connectivities. Progol is well suited to forming SARs for carcinogenicity as it is designed to produce easily understandable rules (structural alerts) for sets of noncongeneric compds. The Progol SAR method was tested by prediction of a set of compds. that have been widely predicted by other SAR methods (the compds. used in the NTP's first round of carcinogenesis predictions). For these compds. no method (human or machine) was significantly more accurate than Progol. Progol was the most accurate method that did not use data from biol. tests on rodents (however, the difference in accuracy is not significant). The Progol predictions were based solely on chem. structure and the results of tests for Salmonella mutagenicity. Using the full NTP database, the prediction accuracy of Progol was estd. to be 63% (±3%) using 5-fold cross validation. A set of structural alerts for carcinogenesis was automatically generated and the chem. rationale for them investigated-these structural alerts are statistically independent of the Salmonella mutagenicity. Carcinogenicity is predicted for the compds. used in the NTP's second round of carcinogenesis predictions. The results for prediction of carcinogenesis, taken together with the previous successful applications of predicting mutagenicity in nitroarom. compds., and inhibition of angiogenesis by suramin analogs, show that Progol has a role to play in understanding the SARs of cancer-related compds.

IT **86-50-0**, Azinphosmethyl **108-46-3**, 1,3-Benzenediol, biological studies **140-56-7**, Fenaminosulf
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(prediction of rodent carcinogenicity bioassays from mol. structure using inductive logic programming)

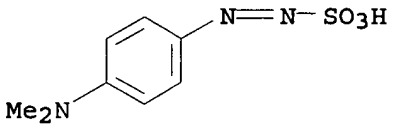
RN 86-50-0 HCAPLUS
CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



RN 140-56-7 HCAPLUS
CN Diazenesulfonic acid, [4-(dimethylamino)phenyl]-, sodium salt (9CI) (CA INDEX NAME)



● Na

CC 4-6 (Toxicology)

IT 50-29-3, biological studies 50-33-9, Phenylbutazone, biological studies 50-55-5, Reserpine 50-81-7, L-Ascorbic acid, biological studies 51-03-6, Piperonyl butoxide 54-31-9, Furosemide 55-31-2 55-38-9, Fenthion 56-38-2, Parathion 56-72-4, Coumaphos 56-81-5D, 1,2,3-Propanetriol, iodo derivs., biological studies 57-06-7, Allyl isothiocyanate 57-41-0, Diphenylhydantoin 58-33-3, Promethazine hydrochloride 58-89-9, Lindane 58-93-5, Hydrochlorothiazide 59-87-0, Nitrofurazone 60-13-9, Amphetamine sulfate 60-51-5, Dimethoate 60-57-1, Dieldrin 61-76-7, Phenylephrine hydrochloride 62-23-7, p-Nitrobenzoic acid 62-73-7, Dichlorvos 64-75-5, Tetracycline hydrochloride 64-77-7, Tolbutamide 67-20-9, Nitrofurantoin 67-72-1 69-53-4, Ampicillin 69-65-8, D-Mannitol 71-43-2, Benzene, biological studies 72-20-8, Endrin 72-43-5, Methoxychlor 72-54-8 72-55-9, biological studies 72-56-0, Di(p-ethylphenyl)dichloroethane 73-22-3, L-Tryptophan, biological studies 74-83-9, biological studies 74-96-4, Bromoethane 75-00-3, Chloroethane 75-09-2, Dichloromethane, biological studies 75-25-2, Tribromomethane 75-27-4, Bromodichloromethane 75-35-4, Vinylidene chloride, biological studies 75-47-8, Iodoform 75-56-9, biological studies 75-65-0, tert-Butyl alcohol, biological studies 76-01-7, Pentachloroethane 76-44-8, Heptachlor 76-87-9, Triphenyltin hydroxide 77-65-6, Carbromal 77-79-2 78-11-5, Pentaerythritol tetranitrate 78-34-2, Dioxathion 78-42-2, Tris(2-ethylhexyl)phosphate 78-59-1, Isophorone 78-87-5, 1,2-Dichloropropane 79-00-5, 1,1,2-Trichloroethane 79-01-6, Trichloroethylene, biological studies 79-11-8, Monochloroacetic acid, biological studies 79-34-5, 1,1,2,2-Tetrachloroethane 80-05-7, biological studies 80-08-0 80-62-6, Methyl methacrylate 81-11-8, 4,4'-Diamino-2,2'-stilbenedisulfonic acid 82-28-0, 1-Amino-2-methylanthraquinone 82-68-8, Pentachloronitrobenzene 83-79-4, Rotenone 85-44-9, 1,3-Isobenzofurandione 85-68-7, Butyl benzyl phthalate 86-30-6, N-Nitrosodiphenylamine **86-50-0**, Azinphosmethyl 86-57-7, 1-Nitronaphthalene 87-29-6, Cinnamyl anthranilate 87-86-5, Pentachlorophenol 88-06-2, 2,4,6-Trichlorophenol 88-96-0, Phthalamide 89-25-8 90-94-8, Michler's ketone 91-08-7, 2,6-Toluene diisocyanate 91-20-3, Naphthalene, biological studies 91-23-6, o-Nitroanisole 91-64-5, Coumarin 91-93-0 92-52-4D, Biphenyl, polybrominated derivs. 94-20-2, Chlorpropamide 94-52-0 95-06-7, Sulfallate 95-14-7, 1,2,3-Benzotriazole 95-50-1, 1,2-Dichlorobenzene 95-74-9, 3-Chloro-p-toluidine 95-79-4, 5-Chloro-o-toluidine 95-80-7, 2,4-Diaminotoluene 95-83-0, 4-Chloro-o-phenylenediamine 96-12-8, 1,2-Dibromo-3-chloropropane 96-13-9, 2,3-Dibromo-1-propanol 96-18-4, 1.2,3-Trichloropropane 96-48-0, γ-Butyrolactone

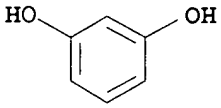
96-69-5, 4,4'-Thiobis(6-tert-butyl-m-cresol) 97-53-0, Eugenol
97-77-8 98-01-1, Furfural, biological studies 98-85-1,
α-Methylbenzyl alcohol 99-55-8, 5-Nitro-o-toluidine
99-56-9, 4-Nitro-o-phenylenediamine 99-57-0, 2-Amino-4-nitrophenol
99-59-2, 5-Nitro-o-anisidine 100-01-6, p-Nitroaniline, biological
studies 100-02-7, p-Nitrophenol, biological studies 100-51-6,
Benzyl alcohol, biological studies 100-52-7, Benzaldehyde,
biological studies 100-80-1, Vinyl m-toluene 101-05-3, Anilazine
101-54-2, N-Phenyl-p-phenylenediamine 101-61-1 101-80-4
101-90-6, Diglycidyl resorcinol ether 102-50-1, m-Cresidine
103-23-1, Di(2-ethylhexyl)adipate 103-33-3, Azobenzene 103-85-5,
1-Phenyl-2-thiourea 103-90-2, 4-Hydroxyacetanilide 105-11-3,
p-Benzoquinone dioxime 105-55-5, N,N'-Diethylthiourea 105-60-2,
biological studies 105-87-3, Geranyl acetate 106-46-7,
1,4-Dichlorobenzene 106-47-8, p-Chloroaniline, biological studies
106-87-6, 4-Vinyl-1-cyclohexene diepoxide 106-88-7,
1,2-Epoxybutane 106-92-3, Allyl glycidyl ether 106-93-4,
1,2-Dibromoethane 107-06-2, 1,2-Dichloroethane, biological studies
107-07-3, 2-Chloroethanol, biological studies 107-21-1,
1,2-Ethanediol, biological studies 108-30-5, biological studies
108-46-3, 1,3-Benzenediol, biological studies 108-60-1,
Bis(2-chloro-1-methylethyl)ether 108-78-1, Melamine, biological
studies 108-88-3, Toluene, biological studies 108-90-7,
Chlorobenzene, biological studies 109-69-3, n-Butyl chloride
113-92-8, Chlorpheniramine maleate 114-86-3, Phenformin
115-07-1, 1-Propene, biological studies 115-28-6, Chlorendic acid
115-32-2, Dicofol 115-96-8, Tris(2-chloroethyl)phosphate
116-06-3, Aldicarb 117-79-3, 2-Aminoanthraquinone 117-81-7,
Di(2-ethylhexyl)phthalate 118-92-3, o-Anthranilic acid 119-34-6,
4-Amino-2-nitrophenol 119-53-9, Benzoin 119-84-6,
3,4-Dihydrocoumarin 119-93-7, 3,3'-Dimethylbenzidine 120-32-1,
o-Benzyl-p-chlorophenol 120-61-6 120-62-7, Piperonyl sulfoxide
120-71-8, p-Cresidine 120-83-2, 2,4-Dichlorophenol 121-14-2,
2,4-Dinitrotoluene 121-19-7, Roxarsone 121-66-4,
2-Amino-5-nitrothiazole 121-69-7, n,N-Dimethylaniline, biological
studies 121-75-5, Malathion 121-79-9, Propyl gallate 121-88-0,
2-Amino-5-nitrophenol 122-66-7, Hydrazobenzene 123-31-9,
1,4-Benzenediol, biological studies 123-91-1, 1,4-Dioxane,
biological studies 124-48-1, Chlorodibromomethane 124-64-1,
Tetrakis(hydroxymethyl) phosphonium chloride 126-72-7,
Tris(2,3-dibromopropyl)phosphate 127-18-4, Tetrachloroethylene,
biological studies 127-69-5, Sulfisoxazole 128-66-5, C.i. Vat
Yellow 4 129-15-7, 2-Methyl-1-nitroanthraquinone 131-17-9,
Diallyl phthalate 132-98-9, Penicillin VK 133-06-2, Captan
133-90-4, Chloramben 134-29-2, o-Anisidine hydrochloride
134-72-5, Ephedrine sulfate 135-20-6, Cupferron 135-88-6,
N-Phenyl-2-naphthylamine 136-40-3, Phenazopyridine hydrochloride
136-77-6, 4-Hexylresorcinol 137-09-7, 2,4-Diaminophenol
dihydrochloride 137-17-7, 2,4,5-Trimethylaniline 137-30-4, Ziram
138-86-3, α-Limonene 139-13-9, Nitrilotriacetic acid
139-65-1 139-94-6, Nithiazide 140-11-4, Benzyl acetate
140-49-8 **140-56-7**, Fenaminosulf 140-88-5, Ethyl acrylate
142-04-1, Aniline hydrochloride 142-46-1, 2,5-Dithiobiurea
147-24-0, Diphenhydramine hydrochloride 148-18-5, Sodium
diethyldithiocarbamate 148-24-3, 8-Hydroxyquinoline, biological
studies 149-30-4, 2-Mercaptobenzothiazole 150-38-9, EdTA
trisodium salt 150-68-5 156-10-5, p-Nitrosodiphenylamine
262-12-4, Dibenzo-p-dioxin 271-89-6, Benzofuran 298-00-0, Methyl
parathion 298-59-9, Methylphenidate hydrochloride 309-00-2,
Aldrin 315-18-4, Mexacarbate 333-41-5, Diazinon 389-08-2,

Nalidixic acid 396-01-0, Triamterene 434-13-9, Lithocholic acid 504-88-1, 3-Nitropropionic acid 509-14-8, Tetranitromethane 510-15-6, Chlorobenzilate 512-56-1, Trimethylphosphate 513-37-1, Dimethylvinyl chloride 532-27-4, 2-Chloroacetophenone 536-33-4, Ethionamide 542-75-6, 1,3-Dichloropropene 555-30-6, Methyldopa 556-52-5, Oxiranemethanol 563-47-3, 3-Chloro-2-methylpropene 569-61-9, C.I. Basic red 9 monohydrochloride 584-84-9 597-25-1, Dimethyl morpholinophosphoramidate 598-55-0, Methyl carbamate 599-79-1, Salicylazosulfapyridine 602-87-9, 5-Nitroacenaphthene 609-20-1, 2,6-Dichloro-p-phenylenediamine 612-82-8, 3,3'-Dimethylbenzidine dihydrochloride 619-17-0 622-97-9, Vinyl p-toluene
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(prediction of rodent carcinogenicity bioassays from mol. structure using inductive logic programming)

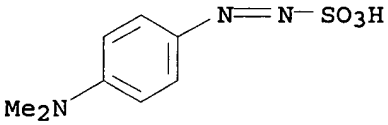
IT 624-18-0, p-Phenylenediamine dihydrochloride 630-20-6, 1,1,1,2-Tetrachloroethane 636-21-5, o-Toluidine hydrochloride 643-22-1, Erythromycin stearate 756-79-6, Dimethyl methylphosphonate 828-00-2, Dimethoxane 842-07-9, C.i. Solvent Yellow 14 868-85-9, Dimethyl hydrogen phosphite 924-42-5, N-Methylolacrylamide 952-23-8 961-11-5 968-81-0, Acetohexamide 989-38-8 999-81-5, 2-Chloroethyltrimethylammonium chloride 1156-19-0, Tolazamide 1163-19-5, Decabromodiphenyl oxide 1212-29-9, n,n'-Dicyclohexylthiourea 1319-77-3D, Hydroxytoluene, Bu derivs. 1330-20-7, Xylene, biological studies 1330-78-5, Tricresyl phosphate 1465-25-4 1490-04-6, Menthol 1582-09-8 1596-84-5, Succinic acid 2,2-dimethylhydrazide 1634-78-2, Malaoxon 1746-01-6, 2,3,7,8-Tetrachlorodibenzo-p-dioxin 1777-84-0, 3-Nitro-p-acetophenetide 1825-21-4, Pentachloroanisole 1836-75-5, Nitrofen 1897-45-6, Chlorothalonil 1918-02-1, Picloram 1936-15-8, C.i. Acid Orange 10 1955-45-9, Pivalolactone 2058-46-0, Oxytetracycline hydrochloride 2164-17-2, Fluometuron 2185-92-4, 2-Biphenylamine hydrochloride 2243-62-1, 1,5-Naphthalenediamine 2425-85-6, C.i. **Pigment** Red 3 2429-74-5, C.i. Direct Blue 15 2432-99-7, 11-Aminoundecanoic acid 2438-88-2, 2,3,5,6-Tetrachloro-4-nitroanisole 2475-45-8, C.i. Disperse Blue 1 2489-77-2, Trimethylthiourea 2698-41-1 2783-94-0 2784-94-3, HC Blue 1 2832-40-8, c.I. Disperse Yellow 3 2835-39-4, Allyl isovalerate 2871-01-4, HC red 3 3165-93-3, 4-Chloro-o-toluidine hydrochloride 3296-90-0, 2,2-Bis(bromomethyl)-1,3-propanediol 3546-10-9, Phenestrin 3567-69-9, C.i. Acid Red 14 5131-60-2, 4-Chloro-m-phenylenediamine 5160-02-1 5307-14-2, 2-Nitro-p-phenylenediamine 6358-85-6 6369-59-1, 2,5-Toluenediamine sulfate 6373-74-6, C.i. Acid Orange 3 6459-94-5, C.i. Acid Red 114 6471-49-4, C.i. **Pigment** Red 23 6959-47-3, 2-Chloromethylpyridine hydrochloride 6959-48-4, 3-Chloromethylpyridine hydrochloride 8001-35-2, Toxaphene 9002-18-0, Agar 9005-65-6, Tween 80 10599-90-3, Chloramine 12789-03-6, Chlordane 13171-21-6, Phosphamidon 13366-73-9, Photodieldrin 13552-44-8, 4,4'-Methylenedianiline dihydrochloride 15481-70-6, 2,6-Toluenediamine dihydrochloride 16873-17-9, Atomic deuterium, biological studies 17026-81-2, 3-Amino-4-ethoxyacetanilide 17924-92-4, Zearalenone 19010-66-3, Lead dimethyldithiocarbamate 20265-96-7, p-Chloroaniline hydrochloride 20265-97-8, p-Anisidine hydrochloride 20325-40-0, 3,3'-Dimethoxybenzidine dihydrochloride 20941-65-5, Ethyl tellurac 22966-79-6, Estradiol mustard 24382-04-5, Malonaldehyde sodium salt 28407-37-6 33229-34-4 33857-26-0, 2,7-Dichlorodibenzo-p-dioxin 34465-46-8, Hexachlorodibenzodioxin 39156-41-7,

2,4-Diaminoanisole sulfate 54150-69-5, 2,4-Dimethoxyaniline hydrochloride 55566-30-8, Tetrakis(hydroxymethyl) phosphonium sulfate 57360-17-5, 3-Amino-9-ethylcarbazole hydrochloride 59820-43-8, HC yellow 4 61702-44-1 89843-47-0, 1H-Benzimidazole, 6-nitro-
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(prediction of rodent carcinogenicity bioassays from mol. structure using inductive logic programming)

L66 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:484720 HCAPLUS
DOCUMENT NUMBER: 117:84720
TITLE: Electrophilicity as measured by Ke: molecular determinants, relationship with other physical-chemical and quantum mechanical parameters, and ability to predict rodent carcinogenicity
AUTHOR(S): Benigni, R.; Cotta-Ramusino, M.; Andreoli, C.; Giuliani, A.
CORPORATE SOURCE: Lab. Comp. Toxicol. Ectoxicol., Ist. Super. Sanita, Rome, Italy
SOURCE: Carcinogenesis (**1992**), 13(4), 547-53
CODEN: CRNGDP; ISSN: 0143-3334
DOCUMENT TYPE: Journal
LANGUAGE: English
AB This paper analyzes electrophilicity data as measured by the Ke system for 205 chems. including both rodent carcinogens and non-carcinogens. Multivariate statistical methods were used. The anal. identified atoms and substructures contributing to electrophilicity, and permitted to establish a theor. method by which the Ke value (electrophilicity) of chems. can be easily estd. In a subset of chems., the Ke parameter was compared with other phys.-chem. and quantum mech. properties: Ke appeared to be mostly correlated with the energy of the LUMO and with the abs. electronegativity. The role of Ke in structure-activity studies was also investigated; in particular, a comparative anal. of the performance of Ke, Salmonella typhimurium and Ashby's structural alerts in predicting carcinogenicity was carried out. The Ke system performed better than the other systems. However, because of the many different mechanisms underlying carcinogenesis, the Ke system cannot predict the potential carcinogenicity of all kinds of chems. It is concluded that the main role of Ke in risk assessment consists in producing a probabilistic est. of the rodent carcinogenicity of the chems.: e.g. a chem. with Ke higher than 3.0 + 1012 M-1 s-1 has nearly 80% probability of being a carcinogen. Such a probability est. can be used to rank the chems. in a priority scale for subsequent and more detailed studies, either theor. or exptl. In view of this, the role of the authors' method for estg. Ke is particularly important as; it gives rapidly and at no cost a chem. classification for risk assessment and priority setting.
IT **108-46-3**, QResorcinol, biological studies **140-56-7**, Fenaminosulf
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(carcinogenicity in rodents of, prediction of, electrophilicity and mol. determinants and quantum mechanics in)
RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



RN 140-56-7 HCAPLUS
CN Diazenesulfonic acid, [4-(dimethylamino)phenyl]-, sodium salt (9CI) (CA INDEX NAME)



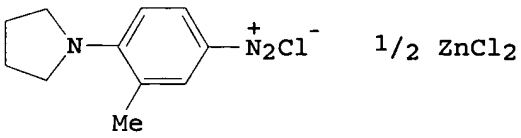
● Na

CC 4-1 (Toxicology)
IT Agrochemicals
Antidepressants
Carcinogens
Detergents
Dyes
Herbicides
Inflammation inhibitors
Insecticides
Pesticides
Pharmaceuticals
Solvents
Surfactants
(carcinogenicity in rodents of, prediction of, electrophilicity and mol. determinants and quantum mechanics in)
IT 50-04-4, Cortisone acetate 50-32-8, Benzo[a]pyrene, biological studies 50-33-9, biological studies 50-49-7, Imipramine 50-53-3, Chlorpromazine, biological studies 50-55-5, Reserpine 50-78-2 50-81-7, L-Ascorbic acid, biological studies 51-03-6, Piperonyl butoxide 51-79-6, Urethane 53-70-3, Dibenz[a,h]anthracene 53-96-3, 2-Acetylaminofluorene 55-18-5, N-Nitrosodiethylamine 56-23-5, Carbon tetrachloride, biological studies 56-53-1, Diethylstilbestrol 56-55-3, Benz[a]anthracene 56-57-5, 4-Nitroquinoline-1-oxide 57-06-7, Allyl isothiocyanate 57-55-6, 1,2-Propanediol, biological studies 57-63-6, Ethynylestradiol 57-83-0, Progesterone, biological studies 57-85-2, Testosterone propionate 57-97-6 58-15-1, Aminopyrine 58-18-4, 17-Methyltestosterone 58-55-9, biological studies 58-89-9, γ-Hexachlorocyclohexane 60-09-3, p-Aminoazobenzene 60-35-5, Acetamide, biological studies 60-51-5 60-57-1, Dieldrin 62-44-2, Phenacetin 62-53-3, Aniline, biological studies 62-55-5, Thioacetamide 62-56-6, Thiourea, biological studies 62-73-7, Dichlorvos 64-17-5, Ethanol, biological studies 64-77-7, Tolbutamide 65-85-0, Benzoic acid, biological studies 67-20-9, Nitrofurantoin 67-64-1, 2-Propanone, biological studies 67-68-5, biological studies 67-72-1, Hexachloroethane 68-12-2, biological studies 69-72-7, biological studies 70-34-8,

2,4-Dinitrofluorobenzene 71-36-3, N-Butanol, biological studies 71-43-2, Benzene, biological studies 74-88-4, Methyl iodide, biological studies 75-47-8, Iodoform 76-01-7, Pentachloroethane 76-44-8, Heptachlor 78-34-2, Dioxathion 78-42-2, Tris(2-ethylhexyl)phosphate 78-59-1, Isophorone 79-01-6, Trichloroethylene, biological studies 79-11-8, Chloracetic acid, biological studies 79-34-5, 1,1,2,2-Tetrachloroethane 79-44-7, Dimethylcarbamylchloride 80-08-0 81-88-9 84-74-2, Dibutylphthalate 85-01-8, Phenanthrene, biological studies 86-00-0, 2-Nitrobiphenyl 86-30-6, N-Nitrosodiphenylamine 86-57-7, 1-Nitronaphthalene 86-73-7, Fluorene 86-74-8, Carbazole 87-29-6, Cinnamyl anthranilate 88-06-2 90-15-3, 1-Naphthalenol 90-43-7, [1,1'-Biphenyl]-2-ol 91-20-3, Naphthalene, biological studies 91-22-5, Quinoline, biological studies 91-59-8, 2-Naphthylamine 92-52-4, Diphenyl, biological studies 92-67-1, p-Aminobiphenyl 92-93-3, 4-Nitrobiphenyl 94-13-3 94-26-8 94-78-0, Phenazopyridine 95-79-4, 5-Chloro-2-toluidine 97-56-3, o-Aminoazotoluene 99-56-9, 4-Nitro-o-phenylenediamine 99-76-3, p-Hydroxybenzoic acid methylester 100-42-5, biological studies 100-44-7, Benzylchloride, biological studies 100-75-4 101-25-7, N,N-Dinitrosopentamethylene tetramine 101-61-1 101-83-7, Dicyclohexylamine 102-50-1 103-23-1, Di(2-ethylhexyl)adipate 103-30-0, trans-Stilbene 103-84-4, Acetanilide 103-90-2, Acetaminophen 104-94-9, p-Anisidine 106-47-8, p-Chloroaniline, biological studies 106-50-3, p-Phenylenediamine, biological studies 106-88-7 106-93-4, Ethylenedibromide 107-07-3, 2-Chloroethanol, biological studies 107-21-1, 1,2-Ethanediol, biological studies 108-05-4, Vinylacetate, biological studies 108-30-5, Succinic anhydride, biological studies **108-46-3**, QResorcinol, biological studies 108-88-3, Toluene, biological studies 110-54-3, n-Hexane, biological studies 110-82-7, Cyclohexane, biological studies 110-86-1, Pyridine, biological studies 111-92-2, Di-N-butylamine 115-28-6, Chlorendic acid 115-32-2 117-81-7, Di(2-ethylhexyl)phthalate 118-92-3, Anthranilic acid 119-53-9, Benzoin 120-12-7, Anthracene, biological studies 120-47-8, p-Hydroxybenzoic acid ethylester 120-62-7, Piperonyl sulfoxide 120-72-9, Indole, biological studies 121-75-5, Malathion 121-79-9, Propyl gallate 123-30-8, p-Aminophenol 123-91-1, 1,4-Dioxane, biological studies 124-40-3, Dimethylamine, biological studies 126-72-7, Tris(2,3-dibromopropyl)phosphate 127-18-4, Tetrachloroethylene, biological studies 127-47-9, Vitamin A acetate 128-37-0, Butylated hydroxytoluene, biological studies 129-00-0, Pyrene, biological studies 133-06-2, Captan 134-32-7, 1-Naphthylamine 135-19-3, 2-Naphthalenol, biological studies 135-88-6, N-Phenyl-2-naphthylamine 137-26-8, Thiram 137-40-6, Sodium propionate 140-11-4, Benzyl acetate 140-49-8 **140-56-7**, Fenaminosulf 140-88-5 148-24-3, 8-Quinolinol, biological studies 150-68-5, Monuron 151-21-3, Sodium lauryl sulfate, biological studies 218-01-9, Chrysene 298-00-0, Methyl parathion 458-37-7, Curcumin 510-15-6, Chlorobenzilate 532-32-1, Sodium benzoate 536-33-4, Ethionamide 551-09-7, N-(1-Naphthyl)ethylenediamine 556-52-5, Glycidol 581-89-5, 2-Nitronaphthalene 584-79-2, Allethrin 592-31-4, N-Butylurea 597-25-1 598-50-5, N-Methylurea 607-57-8, 2-Nitrofluorene 621-64-7, N-Nitrosodipropylamine 630-20-6 637-07-0, Clofibrate 671-16-9, Procarbazine 692-13-7, Buformin 781-43-1, 9,10-Dimethylanthracene 930-55-2, N-Nitrosopyrrolidine 938-73-8 1156-19-0, Tolazamide 1163-19-5, Decabromodiphenyl oxide 1406-18-4, Vitamin E 1464-53-5, 1,2,3,4-Diepoxybutane 1596-84-5

1897-45-6, Chlorothalonil 1934-21-0, Tartrazine 2426-07-5, 1,2,7,8-Diepoxyoctane 2611-82-7, Ponceau 4R 2735-04-8, 2,4-Dimethoxyaniline 2783-94-0, Sunset yellow FCF 2835-39-4 3546-10-9, Phenestrin 4377-33-7, 2-(Chloromethyl)pyridine 4418-26-2, Sodium dehydroacetate 6414-57-9 6441-77-6, Phloxine 7632-00-0, Sodium nitrite 12789-03-6, Chlordane 13366-73-9, Photodieldrin 16423-68-0, Erythrosin 17924-92-4, Zearalenone 22248-79-9, Tetrachlorvinphos 24634-61-5, Potassium sorbate 25013-16-5, Butylated hydroxyanisole 25155-30-0, Sodium dodecyl benzene sulfonate 29418-22-2 30821-43-3 31432-60-7, N-Nitrodiphenylamine 33229-34-4 41674-04-8, Aminobiphenyl 54827-17-7, 3,3',5,5'-Tetramethylbenzidine 56375-33-8, N-Nitrosobutylamine
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(carcinogenicity in rodents of, prediction of, electrophilicity and mol. determinants and quantum mechanics in)

L66 ANSWER 3 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:265347 HCAPLUS
DOCUMENT NUMBER: 116:265347
TITLE: A diazo photosensitive material capable of producing positive and negative images
AUTHOR(S): Tang, Yaling; Qiu, Jiabai; Ma, Jun; Wang, Yanqiao
CORPORATE SOURCE: Inst. Chem., Acad. Sin., Beijing, 100080, Peop. Rep. China
SOURCE: Huaxue Tongbao (**1991**), (10), 37-41
CODEN: HHTPAU; ISSN: 0441-3776
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI



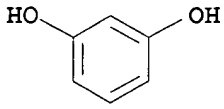
$^1/_2$ $ZnCl_2$

I

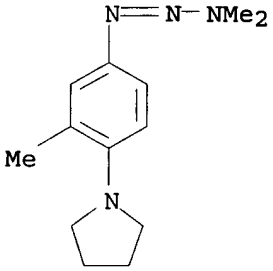
AB A series of azo **dyes** and diazoimine compds. were synthesized using diazo compd. I, and their IR and UV-visible spectra were measured. I was converted to fluoroborate salt to avoid the effect of Zn(OH)2 ppt. on the quality of the produced **dye** images. Azo **dyes** were formed by reaction with a coupling agent in the presence of NaOH, diazoimine compds. by reaction with an amine reagent at pH > 7. The effects of mol. structure of the coupling agents and amine reagents on the products spectral characteristics were compared. It is shown that I can be used either as pos. or neg. imaging material.

IT **108-46-3**, 1,3-Benzenediol, properties
RL: USES (Uses)
(photoimaging material contg. diazo compd. and, spectral characterization of **dye** produced in)

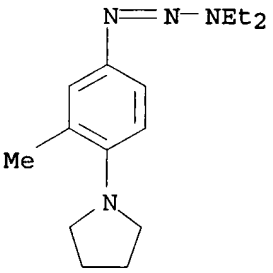
RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



IT **141607-50-3P 141607-51-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and spectral characterization of, photoimaging in relation to)
RN 141607-50-3 HCAPLUS
CN Pyrrolidine, 1-[4-(3,3-dimethyl-1-triazenyl)-2-methylphenyl]- (9CI) (CA INDEX NAME)



RN 141607-51-4 HCAPLUS
CN Pyrrolidine, 1-[4-(3,3-diethyl-1-triazenyl)-2-methylphenyl]- (9CI) (CA INDEX NAME)



CC 74-5 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
IT **Dyes**, azo
(formation of neg. and pos. photoimages of)
IT Infrared spectra
Ultraviolet and visible spectra
(of pos. and neg. diazo **dye** images produced from coupling agents and tetrafluoroborate diazo salt)
IT 92-77-3 **108-46-3**, 1,3-Benzenediol, properties 108-73-6, 1,3,5-Trihydroxybenzene 108-95-2, Phenol, properties 132-68-3 135-61-5 1830-77-9
RL: USES (Uses)
(photoimaging material contg. diazo compd. and, spectral characterization of **dye** produced in)
IT 36422-95-4
RL: USES (Uses)

(photoimaging material contg., spectral characterization of **dye** images produced in)

IT **141607-50-3P 141607-51-4P** 141607-52-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and spectral characterization of, photoimaging in relation to)

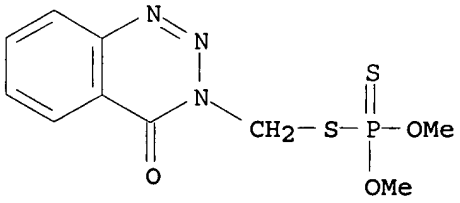
IT 27569-10-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactions of, in formation of diazoimine and diazo **dye** compds., for photoimaging)

L66 ANSWER 4 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:135528 HCAPLUS
DOCUMENT NUMBER: 116:135528
TITLE: Performance-oriented packaging standards; changes to classification, hazard communication, packaging and handling requirements based on UN standards and agency initiative
CORPORATE SOURCE: United States Dept. of Transportation, Washington, DC, 20590-0001, USA
SOURCE: Federal Register (**1990**), 55(246), 52402-729, 21 Dec 1990
CODEN: FEREAC; ISSN: 0097-6326
DOCUMENT TYPE: Journal
LANGUAGE: English

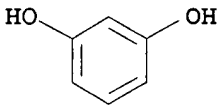
AB The hazardous materials regulations under the Federal Hazardous Materials Transportation Act are revised based on the United Nations recommendations on the transport of dangerous goods. The regulations cover the classification of materials, packaging requirements, and package marking, labeling, and shipping documentation, as well as transportation modes and handling, and incident reporting. Performance-oriented stds. are adopted for packaging for bulk and nonbulk transportation, and SI units of measurement generally replace US customary units. Hazardous material descriptions and proper shipping names are tabulated together with hazard class, identification nos., packing group, label required, special provisions, packaging authorizations, quantity limitations, and vessel stowage requirements.

IT **86-50-0**, Azinphos methyl **108-46-3**, Resorcinol, miscellaneous **591-27-5**, m-Aminophenol
RL: ADV (Adverse effect, including toxicity); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)
(packaging and transport of, stds. for)

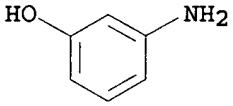
RN 86-50-0 HCAPLUS
CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



RN 591-27-5 HCAPLUS
CN Phenol, 3-amino- (9CI) (CA INDEX NAME)



CC 59-6 (Air Pollution and Industrial Hygiene)
IT **Dyes**
(coal tar, packaging and transport of, stds. for)
IT Adhesives
Alcoholic beverages
Ammunition
Antifreeze substances
Bactericides, Disinfectants, and Antiseptics
Batteries, primary
Blasting gelatin
Bombs (explosives)
Carbon paper
Cartridges
Castor bean
Coating materials
Corrosive substances
Cotton
Creosote
Detonators
Dyes
Dynamite
Electric fuses
Exothermic materials
Explosives
Flavoring materials
Flue dust
Fuel cells
Fuel oil
Fuels, diesel
Fuels, jet aircraft
Fusel oil
Fuses, explosives
Gas oils
Hay
Herbicides
Igniters and Lighters
Insecticides
Lacrimators
Magnetic substances
Matches
Oxidizing agents
Perfumes

Pesticides
Petroleum products
Pharmaceuticals
Photoelectric devices
Poisons
Primers, explosive
Projectiles
Pyrophoric substances
Pyrotechnic compositions
Radioactive substances
Refrigerating apparatus
Rockets
Shale oils
Solvent naphtha
Sprays
Straw
Textiles
Thermoelectric devices
Torpedoes (weapons)
Turpentine
Wood preservatives
(packaging and transport of, stds. for)

IT Pharmaceutical dosage forms
(**tinctures**, packaging and transport of, stds. for)

IT 50-00-0, Formaldehyde, miscellaneous 54-11-5, Nicotine 54-11-5D, Nicotine, compds. 55-63-0, Nitroglycerin 55-68-5, Phenylmercuric nitrate 56-18-8, 3,3'-Iminodipropylamine 56-23-5, miscellaneous 56-38-2, Parathion 57-06-7, Allyl isothiocyanate 57-14-7 57-24-9D, Strychnine, salts 60-00-4, EDTA, miscellaneous 60-24-2 60-29-7, Diethyl ether, miscellaneous 60-34-4, Methylhydrazine 60-57-1, Dieldrin 62-38-4, Phenylmercuric acetate 62-53-3, Aniline, miscellaneous 62-74-8, Sodium fluoroacetate 64-17-5, Ethanol, miscellaneous 64-18-6, Formic acid, miscellaneous 64-18-6D, Formic acid, chloro derivs. 64-19-7, Acetic acid, miscellaneous 64-67-5, Diethyl sulfate 66-25-1, Hexaldehyde 67-56-1, Methanol, miscellaneous 67-63-0, Isopropanol, miscellaneous 67-64-1, Acetone, miscellaneous 67-66-3, Chloroform, miscellaneous 68-11-1, Thioglycolic acid, miscellaneous 68-12-2, N,N-Dimethylformamide, miscellaneous 70-11-1, Phenacyl bromide 70-30-4, Hexachlorophene 71-23-8, n-Propanol, miscellaneous 71-41-0, 1-Pentanol, miscellaneous 71-43-2, Benzene, miscellaneous 71-55-6, 1,1,1-Trichloroethane 74-82-8, Methane, miscellaneous 74-83-9, miscellaneous 74-84-0, Ethane, miscellaneous 74-85-1, Ethylene, miscellaneous 74-86-2, Acetylene, miscellaneous 74-87-3, Methyl chloride, miscellaneous 74-88-4, Methyl iodide, miscellaneous 74-89-5, Methylamine, miscellaneous 74-90-8, Hydrogen cyanide, miscellaneous 74-93-1, Methyl mercaptan, miscellaneous 74-95-3, Dibromomethane 74-96-4, Ethyl bromide 74-97-5, Bromochloromethane 74-98-6, Propane, miscellaneous 75-00-3, Ethyl chloride 75-01-4, miscellaneous 75-02-5, Vinyl fluoride 75-04-7, Ethylamine, miscellaneous 75-05-8, Methyl cyanide, miscellaneous 75-07-0, Acetaldehyde, miscellaneous 75-08-1, Ethyl mercaptan 75-09-2, Dichloromethane, miscellaneous 75-15-0, Carbon disulfide, miscellaneous 75-16-1, Methyl magnesium bromide 75-18-3, Dimethyl sulfide 75-19-4, Cyclopropane 75-20-7, Calcium carbide 75-21-8, Ethylene oxide, miscellaneous 75-21-8 75-25-2, Bromoform 75-26-3, 2-Bromopropane 75-28-5, Isobutane 75-28-5D, Isobutane, mixts. 75-29-6, 2-Chloropropane 75-31-0, Isopropylamine, miscellaneous 75-33-2, Isopropyl mercaptan 75-34-3, 1,1-Dichloroethane

75-35-4, miscellaneous 75-36-5, Acetyl chloride 75-38-7, 1,1-Difluoroethylene 75-39-8, Acetaldehyde ammonia 75-43-4, Dichloromonofluoromethane 75-44-5, Phosgene 75-45-6, Chlorodifluoromethane 75-46-7, Trifluoromethane 75-50-3, Trimethylamine, miscellaneous 75-52-5, Nitromethane, miscellaneous 75-54-7, Methyldichlorosilane 75-55-8, Propylenimine 75-56-9, Propylene oxide, miscellaneous 75-59-2, Tetramethylammonium hydroxide 75-60-5, Cacodylic acid 75-61-6, Dibromodifluoromethane 75-63-8 75-71-8, Dichlorodifluoromethane 75-72-9, Chlorotrifluoromethane 75-73-0, Tetrafluoromethane 75-76-3, Tetramethylsilane 75-77-4, Trimethylchlorosilane, miscellaneous 75-78-5, Dimethyldichlorosilane 75-79-6, Methyltrichlorosilane 75-83-2 75-86-5, Acetone cyanohydrin 75-87-6, Chloral 75-91-2, tert-Butyl hydroperoxide 75-94-5, Vinyltrichlorosilane 76-01-7, Pentachloroethane 76-02-8, Trichloroacetyl chloride 76-03-9, properties 76-05-1, Trifluoroacetic acid, miscellaneous 76-06-2, Chloropicrin 76-06-2D, Chloropicrin, mixts. 76-15-3 76-16-4, Hexafluoroethane 76-19-7, Octafluoropropane 76-22-2, Camphor 77-47-4, Hexachlorocyclopentadiene 77-73-6 77-78-1, Dimethyl sulfate 78-00-2, Tetraethyl lead 78-10-4, Tetraethyl silicate 78-62-6, Dimethyldiethoxysilane 78-67-1, Azodiisobutyronitrile 78-76-2, 2-Bromobutane 78-78-4, Isopentane 78-79-5, Isoprene, miscellaneous 78-81-9, Isobutylamine 78-82-0, Isobutyronitrile 78-83-1, Isobutanol, miscellaneous 78-84-2, Isobutyraldehyde 78-85-3, Methacrylaldehyde 78-87-5, Propylene dichloride 78-89-7, Propylene chlorohydrin 78-90-0, 1,2-Propylenediamine 78-93-3, 2-Butanone, miscellaneous 78-94-4, Methyl vinyl ketone, miscellaneous 78-95-5, Monochloroacetone 79-01-6, Trichloroethylene, miscellaneous 79-03-8, Propionyl chloride 79-04-9, Chloroacetyl chloride 79-06-1, Acrylamide, miscellaneous 79-08-3, Bromoacetic acid 79-09-4, Propionic acid, miscellaneous 79-10-7, 2-Propenoic acid, miscellaneous 79-11-8, Chloroacetic acid, miscellaneous 79-20-9, Methyl acetate 79-21-0, Peroxyacetic acid 79-22-1 79-24-3, Nitroethane 79-29-8, 2,3-Dimethylbutane 79-30-1, Isobutyryl chloride 79-31-2, Isobutyric acid 79-36-7, Dichloroacetyl chloride 79-38-9 79-41-4, miscellaneous 79-42-5 79-43-6, Dichloroacetic acid, miscellaneous 79-44-7, Dimethylcarbamoyl chloride 80-10-4, Diphenyldichlorosilane 80-15-9, Cumene hydroperoxide 80-17-1, Benzene sulfohydrazide 80-47-7, p-Menthane hydroperoxide 80-51-3, Diphenyloxide-4,4'-disulfohydrazide 80-56-8, α-Pinene 80-62-6 81-15-2 82-71-3 85-44-9, 1,3-Isobenzofurandione **86-50-0**, Azinphos methyl 87-68-3, Hexachlorobutadiene 87-90-1 88-17-5, 2-Trifluoromethylaniline 88-72-2, o-Nitrotoluene 88-73-3, o-Chloronitrobenzene 88-74-4, o-Nitroaniline 88-75-5, o-Nitrophenol 88-89-1 89-58-7, p-Nitroxylene 91-17-8, Decahydronaphthalene 91-20-3, Naphthalene, miscellaneous 91-20-3D, Naphthalene, diozonide derivs. 91-22-5, Quinoline, miscellaneous 91-59-8, β-Naphthylamine 91-66-7, N,N-Diethylaniline 92-52-4D, Biphenyl, chloro derivs. 92-52-4D, Biphenyl, halo derivs. 92-59-1, N-Ethyl-N-benzylaniline 92-87-5, Benzidine 93-58-3, Methyl benzoate 94-17-7, p-Chlorobenzoyl peroxide 94-36-0, Benzoyl peroxide, miscellaneous 95-48-7, miscellaneous 95-50-1, o-Dichlorobenzene 95-54-5, o-Phenylenediamine, miscellaneous 95-55-6, o-Aminophenol 95-80-7 95-85-2, 2-Amino-4-chlorophenol 96-12-8, Dibromochloropropane 96-22-0, Diethyl ketone 96-23-1 96-24-2, Glycerol α-monochlorohydrin 96-32-2, Methyl bromoacetate 96-33-3 96-34-4, Methyl chloroacetate 96-37-7,

Methyl cyclopentane 96-41-3, Cyclopentanol 97-62-1, Ethyl isobutyrate 97-63-2 97-64-3, Ethyl lactate 97-72-3, Isobutyric anhydride 97-85-8, Isobutyl isobutyrate 97-86-9 97-88-1 97-95-0 97-96-1, 2-Ethylbutyraldehyde 98-00-0, Furfuryl alcohol 98-01-1, Furfural, miscellaneous 98-07-7, Benzotrichloride 98-08-8, Benzotrifluoride 98-09-9, Benzene sulfonyl chloride 98-12-4, Cyclohexyltrichlorosilane 98-13-5, Phenyltrichlorosilane 98-16-8, 3-Trifluoromethylaniline 98-82-8, Isopropylbenzene 98-83-9, miscellaneous 98-85-1, α-Methylbenzyl alcohol 98-87-3, Benzylidene chloride 98-88-4, Benzoyl chloride 98-94-2 98-95-3, Nitrobenzene, miscellaneous 99-08-1, m-Nitrotoluene 99-09-2, m-Nitroaniline 99-35-4, Trinitrobenzene 99-99-0, p-Nitrotoluene 100-00-5 100-01-6, p-Nitroaniline, miscellaneous 100-02-7, p-Nitrophenol, miscellaneous 100-17-4 100-34-5, Benzene diazonium chloride
RL: ADV (Adverse effect, including toxicity); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)
(packaging and transport of, stds. for)

IT 100-36-7, N,N-Diethylethylenediamine 100-37-8, Diethylaminoethanol 100-39-0, Benzyl bromide 100-41-4, Ethylbenzene, miscellaneous 100-42-5, miscellaneous 100-44-7, Benzyl chloride, miscellaneous 100-47-0, Benzonitrile, miscellaneous 100-50-5, 1,2,3,6-Tetrahydrobenzaldehyde 100-57-2, Phenylmercuric hydroxide 100-61-8, N-Methylaniline, miscellaneous 100-63-0, Phenylhydrazine 100-66-3, Anisole, miscellaneous 100-73-2, Acrolein dimer 101-25-7, N,N'-Dinitrosopentamethylenetetramine 101-68-8 101-77-9, 4,4'-Diaminodiphenyl methane 101-83-7, Dicyclohexylamine 102-69-2, Tripropylamine 102-70-5, Triallylamine 102-81-8, Dibutylaminoethanol 102-82-9, Tributylamine 103-65-1, n-Propylbenzene 103-69-5, N-Ethylaniline 103-71-9, Phenylisocyanate, miscellaneous 103-80-0, Phenylacetyl chloride 103-83-3, Benzyldimethylamine 104-15-4, Toluene sulfonic acid, miscellaneous 104-51-8, Butylbenzene 104-75-6, 2-Ethylhexylamine 104-78-9 104-90-5, 2-Methyl-5-ethylpyridine 105-36-2 105-37-3, Ethyl propionate 105-39-5, Ethyl chloroacetate 105-48-6, Isopropyl chloroacetate 105-54-4, Ethyl butyrate 105-56-6, Ethyl cyanoacetate 105-57-7, Acetal 105-58-8, Diethyl carbonate 105-64-6, Isopropyl peroxydicarbonate 105-74-8, Lauroyl peroxide 106-31-0, Butyric anhydride 106-44-5, p-Cresol, miscellaneous 106-46-7, p-Dichlorobenzene 106-50-3, p-Phenylenediamine, miscellaneous 106-51-4, 2,5-Cyclohexadiene-1,4-dione, miscellaneous 106-63-8, Isobutyl acrylate 106-68-3, Ethyl amyl ketone 106-88-7, 1,2-Butylene oxide 106-89-8, miscellaneous 106-92-3, Allyl glycidyl ether 106-93-4, Ethylene dibromide 106-95-6, Allyl bromide, miscellaneous 106-96-7, 3-Bromopropyne 106-97-8, Butane, miscellaneous 106-97-8D, Butane, mixts. 106-99-0, 1,3-Butadiene, miscellaneous 107-00-6, Ethylacetylene 107-02-8, 2-Propenal, miscellaneous 107-05-1, Allyl chloride 107-06-2, Ethylene dichloride, miscellaneous 107-07-3, Ethylene chlorohydrin, miscellaneous 107-10-8, Propylamine, miscellaneous 107-11-9, Allylamine 107-12-0, Propionitrile 107-13-1, Acrylonitrile, miscellaneous 107-14-2, Chloroacetonitrile 107-15-3, Ethylenediamine, miscellaneous 107-18-6, Allyl alcohol, miscellaneous 107-19-7, Propargyl alcohol 107-20-0, Chloroacetaldehyde 107-25-5, Vinylmethyl ether 107-29-9, Acetaldehyde oxime 107-30-2, Methylchloromethyl ether 107-31-3, Methyl formate 107-37-9, Allyltrichlorosilane 107-49-3, Tetraethyl pyrophosphate 107-70-0 107-71-1, tert-Butyl peroxylacetate 107-72-2, Amyltrichlorosilane 107-81-3,

2-Bromopentane 107-82-4, 1-Bromo-3-methylbutane 107-87-9, Methyl propyl ketone 107-89-1, Aldol 107-92-6, Butyric acid, miscellaneous 108-01-0, Dimethylethanolamine 108-05-4, Acetic acid ethenyl ester, miscellaneous 108-09-8, 1,3-Dimethylbutylamine 108-10-1, Methyl isobutyl ketone 108-11-2, Methyl isobutyl carbinol 108-18-9, Diisopropylamine 108-20-3, Diisopropyl ether 108-21-4, Isopropyl acetate 108-22-5, Isopropenyl acetate 108-23-6, Isopropyl chloroformate 108-24-7, Acetic anhydride 108-31-6, 2,5-Furandione, miscellaneous 108-39-4, miscellaneous 108-45-2, m-Phenylenediamine, miscellaneous **108-46-3**, Resorcinol, miscellaneous 108-67-8, miscellaneous 108-77-0 108-83-8, Diisobutyl ketone 108-84-9 108-86-1, Benzene, bromo-, miscellaneous 108-87-2, Methyl cyclohexane 108-88-3, Toluene, miscellaneous 108-90-7, Chlorobenzene, miscellaneous 108-91-8, Cyclohexylamine, miscellaneous 108-94-1, Cyclohexanone, miscellaneous 108-95-2, Phenol, miscellaneous 108-98-5, Phenyl mercaptan, miscellaneous 109-02-4 109-09-1, 2-Chloropyridine 109-13-7, tert-Butyl peroxyisobutyrate 109-52-4, Valeric acid, miscellaneous 109-53-5, Vinyl isobutyl ether 109-60-4, n-Propyl acetate 109-61-5, n-Propyl chloroformate 109-63-7, Boron trifluoride diethyl etherate 109-65-9, n-Butyl bromide 109-66-0, Pentane, miscellaneous 109-70-6, 1-Chloro-3-bromopropane 109-73-9, n-Butylamine, miscellaneous 109-74-0, Butyronitrile 109-77-3, Malononitrile 109-79-5, Butyl mercaptan 109-86-4, Ethylene glycol monomethyl ether 109-87-5, Methylal 109-89-7, Diethylamine, miscellaneous 109-90-0, Ethyl isocyanate 109-92-2, Vinyl ethyl ether 109-93-3, Divinyl ether 109-94-4, Ethyl formate 109-95-5, Ethyl nitrite 109-99-9, Tetrahydrofuran, miscellaneous 110-00-9, Furan 110-01-0, Tetrahydrothiophene 110-02-1, Thiophene 110-12-3, 5-Methylhexan-2-one 110-16-7, Maleic acid, miscellaneous 110-18-9 110-19-0 110-22-5, Diacetyl peroxide 110-43-0, Amyl methyl ketone 110-49-6 110-54-3, Hexane, miscellaneous 110-58-7, Amylamine 110-62-3, Valeraldehyde 110-66-7, Amyl mercaptan 110-68-9, N-Methylbutylamine 110-69-0, Butyraldoxime 110-71-4, 1,2-Dimethoxyethane 110-74-7, Propyl formate 110-78-1, n-Propyl isocyanate 110-80-5, Ethylene glycol monoethyl ether 110-82-7, Cyclohexane, miscellaneous 110-83-8, Cyclohexene, miscellaneous 110-85-0, Piperazine, miscellaneous 110-86-1, Pyridine, miscellaneous 110-87-2 110-89-4, Piperidine, miscellaneous 110-91-8, Morpholine, miscellaneous 110-96-3, Diisobutylamine 111-15-9, Ethylene glycol monoethyl ether acetate 111-34-2, Butylvinyl ether 111-36-4, n-Butyl isocyanate 111-40-0 111-43-3, Dipropyl ether 111-49-9, Hexamethylenimine 111-65-9, Octane, miscellaneous 111-69-3, Adiponitrile 111-71-7, n-Heptaldehyde 111-76-2, Ethylene glycol monobutyl ether 111-92-2, Di-n-butylamine 112-04-9 112-24-3, Triethylenetetramine 112-57-2 115-07-1, Propylene, miscellaneous 115-10-6, Dimethyl ether 115-11-7, Isobutylene, miscellaneous 115-21-9, Ethyltrichlorosilane 115-25-3, Octafluorocyclobutane 116-14-3, Tetrafluoroethylene, miscellaneous 116-15-4, Hexafluoropropylene 116-16-5, Hexachloroacetone 116-54-1, Methyl dichloroacetate 118-74-1, Hexachlorobenzene 118-96-7, Trinitrotoluene 120-92-3, Cyclopentanone 121-43-7, Trimethyl borate 121-44-8, Triethylamine, miscellaneous 121-45-9, Trimethyl phosphite 121-46-0, 2,5-Norbornadiene 121-69-7, N,N-Dimethylaniline, miscellaneous 121-73-3 121-82-4, Cyclotrimethylenetrinitramine 122-51-0, Ethyl orthoformate 122-52-1, Triethyl phosphite 123-00-2, 4-Morpholinepropanamine 123-15-9 123-19-3, Dipropylketone 123-20-6, Vinyl butyrate

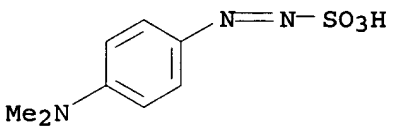
123-23-9, Succinic acid peroxide 123-30-8, p-Aminophenol
123-31-9, Hydroquinone, miscellaneous 123-38-6, Propionaldehyde,
miscellaneous 123-42-2, Diacetone alcohol 123-54-6,
2,4-Pentanedione, miscellaneous 123-62-6, Propionic anhydride
123-63-7, Paraldehyde 123-72-8, Butyraldehyde 123-75-1,
Pyrrolidine, miscellaneous 123-86-4, Butyl acetate 123-91-1,
Dioxane, miscellaneous 124-02-7, Diallylamine 124-09-4,
Hexamethylenediamine, miscellaneous 124-13-0, Octyl aldehyde
124-18-5, n-Decane 124-38-9, Carbon dioxide, miscellaneous
124-40-3, Dimethylamine, miscellaneous 124-41-4, Sodium methylate
124-43-6 124-47-0, Urea nitrate 124-65-2, Sodium cacodylate
126-98-7, Methacrylonitrile 126-99-8, Chloroprene 127-18-4,
Tetrachloroethylene, miscellaneous 127-85-5, Sodium arsanilate
129-79-3 131-52-2, Sodium pentachlorophenate 131-73-7,
Hexanitrodiphenylamine 131-74-8, Ammonium picrate 133-14-2
133-55-1, N,N'-Dinitroso-N,N'-dimethyl terephthalamide 134-32-7,
α-Naphthylamine
RL: ADV (Adverse effect, including toxicity); PEP (Physical,
engineering or chemical process); BIOL (Biological study); PROC
(Process)
(packaging and transport of, stds. for)

IT 138-86-3, Dipentene 138-89-6 139-02-6, Sodium phenolate
140-29-4, Phenylacetonitrile 140-31-8, 1-Piperazineethanamine
140-80-7 140-88-5 141-32-2 141-43-5, Ethanolamine,
miscellaneous 141-57-1, Propyltrichlorosilane 141-59-3,
tert-Octylmercaptan 141-75-3, Butyryl chloride 141-78-6, Ethyl
acetate, miscellaneous 141-79-7, Mesityl oxide 142-04-1, Aniline
hydrochloride 142-29-0, Cyclopentene 142-62-1, Hexanoic acid,
miscellaneous 142-82-5, Heptane, miscellaneous 142-84-7,
Dipropylamine 142-96-1, Dibutyl ether 143-33-9, Sodium cyanide
144-49-0, Fluoroacetic acid 144-62-7D, Ethanedioic acid, salts
146-84-9, Silver picrate 149-74-6, Methylphenyldichlorosilane
151-50-8, Potassium cyanide 151-56-4, Ethylenimine, miscellaneous
156-62-7, Calcium cyanamide 260-94-6, Acridine 283-66-9,
Hexamethylene triperoxide diamine 287-23-0, Cyclobutane
287-92-3, Cyclopentane 291-64-5, Cycloheptane 298-00-0, Methyl
parathion 298-07-7 302-01-2, Hydrazine, miscellaneous
309-00-2, Aldrin 352-93-2, Diethyl sulfide 353-36-6, Ethyl
fluoride 353-42-4, Boron trifluoride dimethyl etherate 353-50-4,
Carbonyl fluoride 353-59-3 354-32-5, Trifluoroacetylchloride
357-57-3, Brucine 360-89-4, Octafluorobut-2-ene 428-59-1,
Hexafluoropropylene oxide 431-03-8, Butanedione 460-19-5,
Cyanogen 462-06-6, Fluorobenzene 462-08-8, m-Aminopyridine
462-95-3, Diethoxymethane 463-04-7, Amyl nitrite 463-49-0,
Propadiene 463-58-1, Carbonyl sulfide 463-71-8, Thiophosgene
463-82-1, 2,2-Dimethylpropane 479-45-8 501-53-1, Benzyl
chloroformate 502-98-7D, salts 503-74-2, Isopentanoic acid
504-24-5, 4-Pyridinamine 504-29-0, 2-Pyridinamine 506-64-9,
Silver cyanide (Ag(CN)) 506-68-3, Cyanogen bromide 506-77-4,
Cyanogen chloride 506-85-4, Fulminic acid 506-93-4, Guanidine
nitrate 506-96-7, Acetyl bromide 507-02-8, Acetyl iodide
507-09-5, Thioacetic acid, miscellaneous 507-70-0, Borneol
509-14-8, Tetranitromethane 512-85-6, Ascaridole 513-35-9,
2-Methyl-2-butene 513-38-2 513-42-8, Methallyl alcohol
513-48-4, 2-Iodobutane 513-86-0, Acetyl methyl carbinol
517-25-9, Trinitromethane 517-92-0, 1,8-Dihydroxy-2,4,5,7-
tetranitroanthraquinone 519-44-8D, 2,4-Dinitroresorcinol, heavy
metal salts 532-27-4, Chloracetophenone 533-51-7, Silver oxalate
534-07-6, 1,3-Dichloroacetone 534-15-6, 1,1-Dimethoxyethane
534-22-5, 2-Methylfuran 535-13-7, Ethyl-2-chloropropionate

540-18-1, Amyl butyrate 540-42-1, Isobutyl propionate 540-54-5, Propyl chloride 540-67-0, Ethyl methyl ether 540-73-8 540-82-9, Ethylsulfuric acid 540-84-1, Isooctane 541-41-3, Ethyl chloroformate 542-55-2, Isobutyl formate 542-62-1, Barium cyanide 542-88-1, Dichlorodimethyl ether, symmetrical 543-27-1, Isobutyl chloroformate 543-59-9, Amyl chloride 544-16-1, Butyl nitrite 544-25-2, Cycloheptatriene 544-97-8, Dimethyl zinc 545-55-1, Tris(1-aziridinyl)phosphine oxide 554-12-1, Methyl propionate 554-84-7, m-Nitrophenol 555-54-4, Magnesium diphenyl 556-24-1, Methyl isovalerate 556-56-9, Allyl iodide 556-61-6, Methyl isothiocyanate 556-88-7 556-89-8, Nitrourea 557-17-5, Methyl propyl ether 557-19-7, Nickel cyanide (Ni(CN)2) 557-20-0, Diethylzinc 557-21-1, Zinc cyanide 557-31-3, Allyl ethyl ether 557-40-4, Diallylether 557-98-2, 2-Chloropropene 558-13-4, Carbon tetrabromide 563-45-1, 3-Methyl-1-butene 563-46-2, 2-Methyl-1-butene 563-47-3, Methyl allyl chloride 563-80-4, 3-Methylbutan-2-one 578-54-1, 2-Ethylaniline 578-94-9, Diphenylamine chloroarsine 582-61-6, Benzoyl azide 583-15-3, Mercury benzoate 584-79-2, Allethrin 585-79-5, 1-Bromo-3-nitrobenzene 586-62-9, Terpinolene 587-85-9D, compds. 590-01-2, Butylpropionate 590-36-3, 2-Methylpentan-2-ol **591-27-5**, m-Aminophenol 591-87-7, Allyl acetate 591-89-9, Mercuric potassium cyanide 592-01-8, Calcium cyanide 592-05-2, Lead cyanide (Pb(CN)2) 592-34-7, n-Butylchloroformate 592-41-6, 1-Hexene, miscellaneous 592-55-2, 2-Bromoethyl ethyl ether 592-63-2 592-84-7, n-Butylformate 593-53-3, Methyl fluoride 593-60-2, Vinyl bromide 593-89-5, Methyldichloroarsine 594-42-3, Perchloromethylmercaptan 594-72-9, 1,1-Dichloro-1-nitroethane 598-14-1, Ethyldichloroarsine 598-21-0, Bromoacetyl bromide 598-31-2, Bromoacetone 598-57-2, Methyl nitramine 598-57-2D, Methyl nitramine, metal salts 598-58-3, Methyl nitrate 598-73-2, Bromotrifluoroethylene 598-78-7, α-Chloropropionic acid 598-99-2, Methyl trichloroacetate 602-96-0, 1,3,5-Trimethyl-2,4,6-trinitrobenzene 602-99-3, Trinitro-m-cresol 602-99-3D, Methyl picric acid, heavy metal salts 608-50-4, 2,4-Dinitro-1,3,5-trimethylbenzene 610-38-8, 4-Bromo-1,2-dinitrobenzene 616-38-6, Dimethyl carbonate 616-74-0D, 4,6-Dinitroresorcinol, heavy metal salts 617-37-8 617-50-5, Isopropyl isobutyrate 617-89-0, Furfurylamine 619-97-6, Benzene diazonium nitrate 620-05-3, Benzyl iodide 622-44-6, Phenylcarbylamine chloride 622-45-7, Cyclohexyl acetate 623-42-7, Methyl butyrate 623-87-0, Glycerol-1,3-dinitrate 624-61-3, Dibromoacetylene 624-74-8, Diiodoacetylene 624-83-9, Methyl isocyanate 624-91-9, Methyl nitrite 624-92-0, Dimethyl disulfide 625-76-3, Dinitromethane 626-67-5, 1-Methylpiperidine 627-13-4, n-Propyl nitrate 627-30-5 627-63-4, Fumaryl chloride 628-28-4, Butyl methyl ether 628-32-0, Ethyl propyl ether 628-63-7, Amyl acetate 628-81-9, Ethyl butyl ether 628-86-4, Mercury fulminate 628-92-2, Cycloheptene 628-96-6, Ethylene glycol dinitrate 629-13-0, 1,2-Diazidoethane 629-14-1 629-20-9, Cyclooctatetraene 630-08-0, Carbon monoxide, miscellaneous 630-72-8, Trinitroacetonitrile 637-78-5, Isopropyl propionate 638-11-9, Isopropyl butyrate 638-29-9, Valeryl chloride 638-49-3, Amyl formate 641-16-7, 2,3,4,6-Tetranitrophenol 644-31-5, Acetyl benzoyl peroxide 644-97-3, Phenyl phosphorus dichloride 645-55-6, N-Nitroaniline 646-06-0, Dioxolane 674-81-7, Nitrosoguanidine 674-82-8, Diketene 676-83-5, Methyl phosphonous dichloride 676-97-1, Methyl phosphonic dichloride 676-98-2, Methyl phosphonothioic dichloride 677-71-4, Hexafluoroacetone hydrate 681-84-5, Methyl orthosilicate

684-16-2, Hexafluoroacetone 693-21-0, Diethylene glycol dinitrate 694-05-3, 1,2,3,6-Tetrahydropyridine 757-58-4, Hexaethyl tetraphosphate 762-12-9, Decanoyl peroxide 762-13-0, Pelargonyl peroxide 762-16-3 765-34-4, Glycidaldehyde 766-09-6, 1-Ethylpiperidine 771-29-9, Tetralin hydroperoxide 776-74-9, Diphenylmethyl bromide 814-78-8, Methyl isopropenyl ketone 822-06-0 831-52-7, Sodium picramate 883-40-9, Diazodiphenylmethane 918-37-6, Hexanitroethane 918-54-7, Trinitroethanol 926-63-6 926-64-7, 2-Dimethylaminoacetonitrile 928-65-4, Hexyltrichlorosilane 929-06-6, 2-(2-Aminoethoxy)ethanol 993-00-0, Methylchlorosilane 993-12-4 993-43-1, Ethyl phosphonothioic dichloride
RL: ADV (Adverse effect, including toxicity); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)
(packaging and transport of, stds. for)

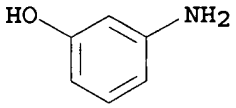
L66 ANSWER 5 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:145157 HCAPLUS
DOCUMENT NUMBER: 108:145157
TITLE: Salmonella mutagenicity tests: IV. Results from the testing of 300 chemicals
AUTHOR(S): Zeiger, Errol; Anderson, Beth; Haworth, Steve; Lawlor, Timothy; Mortelmans, Kristien
CORPORATE SOURCE: Cell. Genet. Toxicol. Branch, Natl. Inst. Environ. Health Sci., Research Triangle Park, NC, USA
SOURCE: Environmental and Molecular Mutagenesis (**1988**), 11(Suppl. 12), 1-157
CODEN: EMMUEG; ISSN: 0893-6692
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Three hundred chem. were tested for mutagenicity, under code, in S. typhimurium, using a preincubation protocol. All tests were performed in the absence of exogenous metabolic activation, and in the presence of liver S-9 from Aroclor-induced male Sprague-Dawley rats and Syrian hamsters. The results and data from these tests are presented.
IT **140-56-7 591-27-5**, m-Aminophenol **4342-03-4**, Dacarbazine
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(mutagenicity of, in Ames test)
RN 140-56-7 HCAPLUS
CN Diazenesulfonic acid, [4-(dimethylamino)phenyl]-, sodium salt (9CI) (CA INDEX NAME)



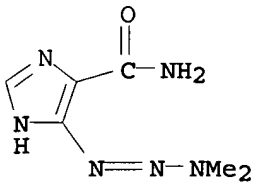
● Na

RN 591-27-5 HCAPLUS

CN Phenol, 3-amino- (9CI) (CA INDEX NAME)



RN 4342-03-4 HCAPLUS
CN 1H-Imidazole-4-carboxamide, 5-(3,3-dimethyl-1-triazenyl)- (9CI) (CA INDEX NAME)



CC 4-6 (Toxicology)
IT 50-55-5, Reserpine 50-78-2, Acetylsalicylic acid 50-81-7, biological studies 55-18-5, N-Nitrosodiethylamine 55-21-0, Benzamide 56-23-5, biological studies 56-35-9, Hexabutyl distannoxane 56-54-2, Quinidine 56-93-9, Benzyltrimethyl ammonium chloride 57-63-6 57-83-0, Progesterone, biological studies 58-54-8, Ethacrynic acid 58-55-9, Theophylline, biological studies 58-90-2, 2,3,4,6-Tetrachlorophenol 59-96-1, Phenoxybenzamine 61-82-5, 3-Amino-1,2,4-triazole 62-56-6, Thiourea, biological studies 62-73-7, Dichlorvos 65-85-0, biological studies 75-36-5 75-86-5, 2-Hydroxy-2-methyl-propanenitrile 75-87-6 78-63-7, 2,5-Dimethyl-2,5-bis(tert-butylperoxy)hexane 78-83-1, biological studies 78-88-6, 2,3-Dichloro-1-propene 79-00-5 79-15-2, N-Bromoacetamide 79-21-0 80-43-3, Dicumyl peroxide 80-46-6 80-47-7, p-Menthane hydroperoxide 81-14-1, Musk ketone 82-28-0, 1-Amino-2-methylanthraquinone 83-89-6, Quinacrine 84-65-1, Anthraquinone 85-01-8, biological studies 85-98-3, N,N'-Diethylcarbanilide 86-00-0 86-30-6 87-29-6, Cinnamyl anthranilate 87-59-2, 2,3-Xylidine 87-62-7, 2,6-Xylidine 88-21-1, o-Amino benzenesulfonic acid 88-23-3 88-88-0, Picryl chloride 89-40-7, 4-Nitrophthalimide 89-78-1 90-30-2, N-Phenyl-1-naphthylamine 91-59-8, 2-Naphthylamine 91-66-7, N,N-Diethyl aniline 91-68-9, 3-Diethylaminophenol 92-59-1, N-Ethyl-N-phenyl benzylamine 93-05-0, N,N-Diethyl-p-phenylenediamine 94-36-0, Benzoyl peroxide, biological studies 94-70-2, o-Phenetidine 95-54-5, biological studies 95-64-7, 3,4-Xylidine 95-68-1, 2,4-Xylidine 95-78-3, 2,5-Xylidine 95-83-0, 4-Chloro-o-phenylenediamine 95-84-1, 2-Amino-4-methylphenol 95-85-2, 2-Amino-4-chlorophenol 96-12-8, 1,2-Dibromo-3-chloropropane 96-23-1, 1,3-Dichloro-2-propanol 96-24-2, 3-Chloro-1,2-propanediol 96-67-3 96-91-3, 2-Amino-4,6-dinitrophenol 97-18-7, 2,2'-Thiobis(4,6-dichlorophenol) 97-24-5, 2,2'-Thiobis(4-chlorophenol) 98-07-7 98-08-8 98-11-3, biological studies 98-37-3 99-07-0, 3-Dimethylaminophenol 99-82-1, p-Menthane 100-22-1, N,N,N',N'-Tetramethyl-p-phenylenediamine 100-42-5, biological studies 100-47-0, biological studies 100-61-8, biological

studies 101-05-3, Anilazine 101-18-8 101-70-2, 4,4'-Dimethoxydiphenylamine 101-77-9 101-80-4, 4,4'-Oxydianiline 101-96-2, N,N'-Di-sec-butyl-p-phenylenediamine 102-01-2, Acetoacetanilide 102-28-3, m-Aminoacetanilide 102-50-1, m-Cresidine 103-69-5, N-Ethyl aniline 103-70-8 103-84-4 104-75-6, 2-Ethylhexylamine 104-85-8, p-Tolunitrile 106-20-7 106-40-1, p-Bromoaniline 106-50-3, biological studies 107-12-0 107-16-4 107-35-7 108-45-2, biological studies 108-69-0, 3,5-Xylidine 109-57-9, Allylthiourea 109-77-3 110-05-4, Di-tert-butyl peroxide 110-17-8, biological studies 110-26-9, N,N'-Methylene-bis-acrylamide 110-61-2 110-88-3, biological studies 111-42-2D, reaction product with coconut oil acid 111-69-3 112-80-1D, reaction product with ethanolamine 114-83-0, 1-Acetyl-2-phenylhydrazine 116-06-3 119-15-3, 4-(2,4-Dinitroanilino)phenol 119-93-7, 3,3'-Dimethylbenzidine 120-37-6, 3-Ethylamino-4-methylphenol 120-71-8, p-Cresidine 120-78-5, 2,2'-Dithiobisbenzothiazole 121-47-1, m-Amino benzenesulfonic acid 121-57-3, p-Amino benzenesulfonic acid 122-39-4, biological studies 122-80-5, p-Aminoacetanilide 123-05-7 123-30-8, p-Aminophenol 124-07-2, biological studies 124-30-1, Octadecylamine 126-27-2, Oxethazaine 127-19-5 127-69-5, Sulfisoxazole 127-85-5, Sodium arsanilate 133-18-6, Phenethyl anthranilate 134-31-6, 8-Hydroxyquinoline sulfate 134-32-7, 1-Naphthylamine 134-72-5, Ephedrine sulfate 135-88-6, N-Phenyl-2-naphthylamine 137-89-3, Bis(2-ethylhexyl)isophthalate 139-65-1, 4,4'-Thiodianiline 140-29-4, Phenylacetonitrile **140-56-7** 143-07-7, biological studies 143-07-7D, reaction product with diethanolamine 143-16-8, Dihexylamine 143-27-1, Hexadecylamine 148-24-3, 8-Hydroxyquinoline, biological studies 148-79-8, Thiabendazole 149-57-5, 2-Ethylhexanoic acid 150-38-9 156-43-4, p-Phenetidine 156-59-2 262-20-4 301-12-2, Metasystox-R 303-47-9, Ochratoxin A 309-36-4, Sodium methohexital 333-41-5, Diazinon 334-48-5 366-70-1 367-25-9, 2,4-Difluoroaniline 389-08-2, Nalidixic acid 434-13-9, Lithocholic acid 480-81-9, Seneciphylline 496-72-0, 3,4-Diaminotoluene 503-30-0 504-88-1, 3-Nitropropionic acid 527-85-5, 2-Methylbenzamide 528-74-5, Dichloromethotrexate 529-19-1, o-Tolunitrile 529-20-4, o-Tolualdehyde 532-28-5 536-33-4, Ethionamide 540-51-2 544-63-8, biological studies 551-06-4, α-Naphthyl isothiocyanate 555-30-6, Methyl DOPA 555-48-6, 2-Aminoacetanilide 563-47-3, 3-Chloro-2-methylpropene **591-27-5**, m-Aminophenol 598-55-0, Methyl carbamate 599-79-1, Salicylazosulfapyridine 602-60-8, 9-Nitroanthracene 603-54-3 610-66-2, o-Nitrophenyl acetonitrile 613-93-4, N-Methylbenzamide 615-05-4, 2,4-Diaminoanisole 616-23-9, 2,3-Dichloro-1-propanol 620-22-4, m-Tolunitrile 621-31-8, 3-Ethylaminophenol 621-33-0, m-Phenetidine 621-42-1, N-Acetyl-m-aminophenol 623-30-3, β-2-Furyl acrolein 637-62-7, p-Quinone monooxime 645-62-5, 2-Ethyl-2-hexenal 823-40-5, 2,6-Diaminotoluene 842-07-9, Solvent yellow 14 881-03-8, 1-Nitro-2-methylnaphthalene 924-42-5, N-Methylolacrylamide 931-97-5, Cyclohexanone cyanohydrin 935-95-5, 2,3,5,6-Tetrachlorophenol 1116-54-7, N-Nitrosodiethanolamine 1143-38-0, Anthralin 1156-19-0, Tolazamide 1187-42-4, Diaminomaleonitrile 1212-29-9, N,N'-Dicyclohexylthiourea 1291-32-3, Zirconocene dichloride 1328-53-6, **Pigment** green 7 1634-78-2, Malaoxon 1875-92-9, Benzyldimethyl ammonium chloride 1912-24-9, Atrazine 1929-82-4, 2-Chloro-6-(trichloromethyl)pyridine 1936-15-8, Acid orange 10 1972-08-3 2039-87-4, o-Chlorostyrene 2163-80-6

2164-17-2, Fluometuron 2179-59-1, Allyl propyl disulfide
2185-92-4 2461-15-6, 2-Ethylhexyl glycidyl ether 2475-45-8,
Disperse blue 1 2493-84-7, p-n-Octyloxybenzoic acid 2528-36-1,
Dibutyl phenyl phosphate 2783-94-0 2784-94-3 2832-40-8,
Disperse yellow 3 2835-95-2, 3-Amino-6-methylphenol 2871-01-4
2941-64-2 3129-91-7, Dicyclohexylamine nitrite 3268-87-9
3319-31-1 3333-52-6, Tetramethyl succinonitrile 3682-19-7
3689-24-5 4080-31-3, N-(3-Chloroallyl)hexaminium chloride
4196-87-6 **4342-03-4**, Dacarbazine 4345-03-3,
D-α-Tocopheryl succinate 4424-06-0 4901-51-3,
2,3,4,5-Tetrachlorophenol 5131-58-8
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(mutagenicity of, in Ames test)

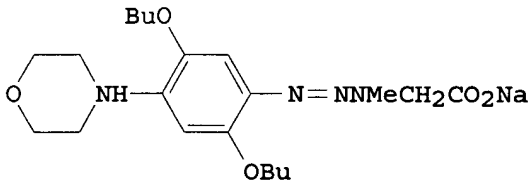
IT 5160-02-1 5307-14-2, 2-Nitro-p-phenylenediamine 5397-31-9,
3-((2-Ethylhexyl)oxy)propylamine 5466-84-2, 4-Nitrophthalic
anhydride 6201-87-2, 5-Amino-3-sulfosalicylic acid 6358-07-2
6358-09-4 6358-20-9, 5-Diethylamino-2-nitrosophenol 6358-23-2
6358-31-2, **Pigment** yellow 74 6369-59-1 6373-74-6, Acid
orange 3 6428-94-0, Direct violet 32 7195-43-9 7206-76-0
7446-34-6, Selenium sulfide 7492-66-2, Citral diethyl acetal
7647-14-5, biological studies 8003-22-3 8005-02-5, Solvent black
7 9002-86-2 10213-75-9 11084-85-8, Chlorinated trisodium
phosphate 11097-69-1, Aroclor 1254 11099-03-9, Solvent black 5
12122-67-7, Zineb 12225-21-7 13098-39-0, Hexafluoroacetone
sesquihydrate 13366-73-9, Photodieldrin 13463-67-7, biological
studies 13552-21-1 15110-74-4 15242-96-3, Stearatochromic
chloride complex 16091-18-2 16452-01-0 17341-40-1,
1,1-Dimethyl-1-(2-hydroxypropylamine)methacrylimide 17369-59-4,
3-Propylidene phthalide 17804-35-2, Benomyl 21739-91-3,
Cytembena 22224-92-6, Phenamiphos 23246-96-0, Riddelliine
24815-24-5, Rescinnamine 25155-25-3 25852-70-4,
Butyltin-tris(isooctylmercaptoacetate) 26227-73-6 26266-68-2,
2-Ethylhexenal 26401-97-8 26763-63-3, Diphenylurea 28108-99-8,
Isopropylphenyl diphenyl phosphate 28906-50-5, Methyl
glutaronitrile 29350-73-0, Cadinene 29385-43-1 29964-84-9,
Isodecyl methacrylate 31551-45-8 33229-34-4 34807-41-5,
Mezerein 37224-57-0, Zinc potassium chromate 38638-05-0,
Nonylphenyl diphenyl phosphate 38848-76-9 54827-17-7,
3,3',5,5'-Tetramethylbenzidine
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(mutagenicity of, in Ames test)

L66 ANSWER 6 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:59011 HCAPLUS
DOCUMENT NUMBER: 106:59011
TITLE: Diazo heat-sensitive recording materials of sublimation-transferring type
INVENTOR(S): Yabuta, Kenji; Morishita, Sadao
PATENT ASSIGNEE(S): Mitsubishi Paper Mills, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

JP 61144388	A2	19860702	JP 1984-268072	198412 18 <--
PRIORITY APPLN. INFO.:			JP 1984-268072	198412 18 <--

GI

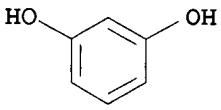


I

AB The title materials comprise transfer sheets with a layer contg. a sublimating coupler and a binder with high softening point and image receptor sheets with a layer contg. a diazoamino compd. forming a **dye** with the coupler. The materials are able to reproduce variable gradations in variable **colors** and are used repeatedly without deterioration in **color** d. Thus, a receptor sheet was prepd. using I and poly(vinyl alc.) and a transfer sheet was prepd. using Et cellulose and resorcinol. Both sheets were superposed and applied to a thermal block at 150° for 5 s, giving a **color** image on the receptor sheet with high **color** d.

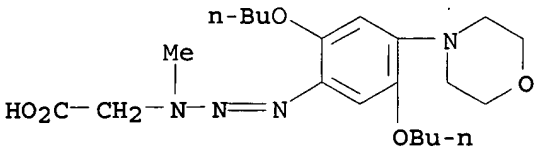
IT **108-46-3**, Resorcinol, uses and miscellaneous
RL: USES (Uses)
(diazo thermal recording material with image receptor layer contg. diazoamino compd. and transfer layer contg. binder and)

RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



IT **62497-78-3**
RL: USES (Uses)
(diazo thermal recording material with image receptor layer contg., and transfer layer contg. sublimating coupler)

RN 62497-78-3 HCAPLUS
CN Acetic acid, [3-[2,5-dibutoxy-4-(4-morpholinyl)phenyl]-1-methyl-2-triazenyl]-, monosodium salt (9CI) (CA INDEX NAME)



● Na

IC ICM B41M005-18
ICS B41M005-26
CC 74-12 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
IT 90-43-7, o-Phenylphenol **108-46-3**, Resorcinol, uses and miscellaneous 135-19-3, β-Naphthol, uses and miscellaneous
RL: USES (Uses)
(diazo thermal recording material with image receptor layer contg. diazoamino compd. and transfer layer contg. binder and)
IT **62497-78-3**
RL: USES (Uses)
(diazo thermal recording material with image receptor layer contg., and transfer layer contg. sublimating coupler)

L66 ANSWER 7 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:41707 HCAPLUS
DOCUMENT NUMBER: 106:41707
TITLE: Diazo heat-sensitive recording materials of sublimation-transferring type
INVENTOR(S): Yabuta, Kenji; Morishita, Sadao
PATENT ASSIGNEE(S): Mitsubishi Paper Mills, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61144389	A2	19860702	JP 1984-268073	19841218

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PRIORITY APPLN. INFO.: JP 1984-268073 19841218

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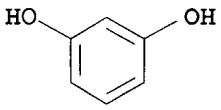
AB The title materials comprise transfer sheets with layers contg. sublimating couplers and binders with high softening points and image receptor sheets having layers contg. org. basic compds. and diazosulfonates forming **dyes** by reaction with the couplers. The materials provide variable gradations in variable **colors** and are used repeatedly without deterioration in **color** d. Thus, a receptor sheet was prepd. using Na 4-(4'-trimercapto)-2,5-diethoxybenzenediazosulfonate and

(C6H11NH)2C:NPh and a transfer sheet was prepd. using resorcinol and Et cellulose. The receptor was irradiated with a Xe-flash (5 J/cm2) to activate, superposed with the transfer sheet, applied to a thermal block at 120° for 3 s to obtain an image on the receptor, irradiated with a fluorescent lamp for 50 s to decompd. the diazosulfonate on the non-image part. The resulting image showed high **color** d.

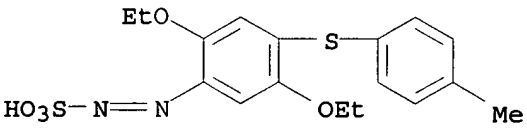
IT **108-46-3**, Resorcinol, uses and miscellaneous
RL: USES (Uses)
(diazo thermal recording material with image receptor contg. org. basic compd. and diazosulfonate and transfer layer contg.)

RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



IT **36429-19-3**
RL: USES (Uses)
(diazo thermal recording material with image receptor layer contg., and transfer layer contg. sublimating coupler)

RN 36429-19-3 HCAPLUS
CN Diazenesulfonic acid, [2,5-diethoxy-4-[(4-methylphenyl)thio]phenyl]-, sodium salt (9CI) (CA INDEX NAME)



● Na

IC ICM B41M005-18
ICS B41M005-26

CC 74-12 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

IT **108-46-3**, Resorcinol, uses and miscellaneous
RL: USES (Uses)
(diazo thermal recording material with image receptor contg. org. basic compd. and diazosulfonate and transfer layer contg.)

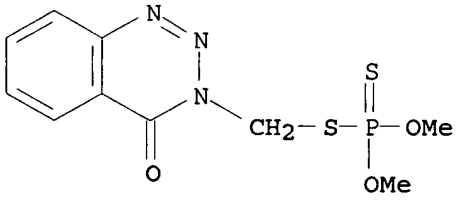
IT **36429-19-3**
RL: USES (Uses)
(diazo thermal recording material with image receptor layer contg., and transfer layer contg. sublimating coupler)

L66 ANSWER 8 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:597481 HCAPLUS
DOCUMENT NUMBER: 101:197481
TITLE: Determination of sources of selected substances and their retention in sewage sludge
AUTHOR(S): Arendt, Gerhard; Eggersdorfer, Rolf; Faltin,

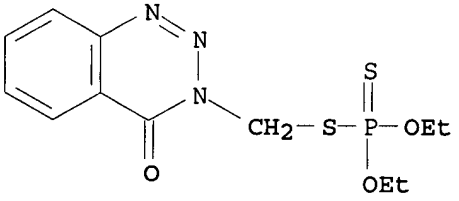
Marta; Frische, Rainer; Haag, Franz; Lichtwer, Liselotte; Rippen, Gerd; Steinsiek, Eckart
CORPORATE SOURCE: Battelle-Inst. e.V., Frankfurt/Main, Fed. Rep. Ger.
SOURCE: Forschungsber. - Bundesminist. Forsch. Technol., Technol. Forsch. Entwickl. (1983), BMFT-FB-T 83-281, 136 pp.
CODEN: BFTEAJ; ISSN: 0340-7608
DOCUMENT TYPE: Report
LANGUAGE: German
AB A method is described which permits identification of groups of substances (.apprx.370 compds.) present in the technosphere and representing a potential health hazard in the agricultural use of sewage sludges. The multi-stage evaluation procedure includes (1) characterization of the substances, (2) investigation of the technosphere, (3) collection of anal. data, (4) theor. consideration, and (5) final evaluation of the substances.

IT **86-50-0 2642-71-9**
RL: POL (Pollutant); OCCU (Occurrence)
(detn. of sources and detention of, in sewage sludges in agricultural uses, health hazard in relation to)

RN 86-50-0 HCAPLUS
CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)

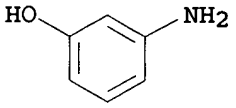


RN 2642-71-9 HCAPLUS
CN Phosphorodithioic acid, O,O-diethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



IT **591-27-5**
RL: POL (Pollutant); OCCU (Occurrence)
(detn. of sources and retention of, in sewage sludges in agricultural uses, health hazard in relation to)

RN 591-27-5 HCAPLUS
CN Phenol, 3-amino- (9CI) (CA INDEX NAME)



CC 60-6 (Waste Treatment and Disposal)
Section cross-reference(s): 19, 59, 61

IT **Pigments**
(detn. of sources and detention of, in sewage sludges in agricultural uses, health hazard in relation to)

IT **Dyes**
(org., detn. of sources and detention of, in sewage sludges in agricultural uses, health hazard in relation to)

IT 50-00-0, biological studies 50-32-8, biological studies 51-28-5, analysis 52-68-6 55-18-5 55-38-9 56-38-2 57-13-6, analysis 59-89-2 60-51-5 62-73-7 62-75-9 63-25-2 67-64-1, biological studies 75-05-8, biological studies 75-07-0, biological studies 75-86-5 75-87-6 78-00-2 78-59-1 78-82-0 78-93-3, biological studies **86-50-0** 88-15-3 88-72-2 90-02-8, biological studies 91-20-3, biological studies 91-20-3D, chloro derivs. 91-22-5, biological studies 91-64-5 95-15-8 96-33-3 98-01-1, biological studies 98-48-6 98-86-2, biological studies 98-95-3, biological studies 99-99-0 100-47-0, biological studies 100-52-7, biological studies 104-15-4, analysis 105-45-3 107-02-8, biological studies 108-10-1 108-95-2D, alkyl derivs., ethers with polyethylene glycol 108-98-5, biological studies 109-86-4 110-49-6 110-80-5 111-15-9 111-44-4 111-55-7 111-76-2 115-29-7 115-86-6 115-96-8 119-61-9, biological studies 120-12-7, biological studies 120-61-6 120-78-5 121-14-2 122-14-5 122-79-2 123-38-6, biological studies 123-91-1, analysis 126-33-0 126-72-7 128-37-0, analysis 130-20-1 142-96-1 149-30-4 150-68-5 298-00-0 298-04-4 330-54-1 330-55-2 333-41-5 574-93-6 588-59-0 606-20-2 610-39-9 628-96-6 1113-02-6 1330-78-5 1746-81-2 **2642-71-9** 3766-60-7 7397-62-8 7440-38-2D, compds. 7704-34-9D, compds. 7723-14-0D, compds. 8022-00-2 8062-15-5 10265-92-6 11067-81-5 11084-05-2 16984-48-8, biological studies 19937-59-8 24017-47-8 25496-01-9 25791-96-2 26523-78-4 27176-87-0 37953-05-2 63637-46-7
RL: POL (Pollutant); OCCU (Occurrence)
(detn. of sources and detention of, in sewage sludges in agricultural uses, health hazard in relation to)

IT 50-29-3, biological studies 50-78-2 56-23-5, biological studies 56-81-5, biological studies 57-10-3, analysis 57-11-4, biological studies 57-55-6, biological studies 59-50-7 60-00-4, analysis 60-57-1 62-53-3, biological studies 64-17-5, biological studies 65-85-0, biological studies 67-56-1, biological studies 67-63-0, biological studies 67-66-3, biological studies 67-72-1 69-72-7, biological studies 71-23-8, biological studies 71-36-3, biological studies 71-41-0, biological studies 71-43-2, biological studies 71-55-6 72-20-8 72-43-5 72-54-8 72-55-9, biological studies 75-01-4, biological studies 75-09-2, biological studies 75-34-3 75-35-4, analysis 75-99-0 76-44-8 77-47-4 77-73-6 77-92-9, biological studies 78-83-1, biological studies 79-01-6, analysis 79-11-8, biological studies 79-20-9 79-34-5 80-05-7, analysis 82-68-8 84-66-2 84-74-2 84-76-4 84-77-5 85-68-7 87-68-3

87-86-5 88-06-2 88-73-3 88-85-7 88-89-1 88-99-3,
biological studies 88-99-3D, esters 90-04-0 90-43-7 91-23-6
92-52-4D, chloro derivs. 92-87-5 93-65-2 93-76-5 94-74-6
94-75-7, biological studies 95-47-6, biological studies 95-48-7,
biological studies 95-49-8 95-50-1 95-51-2 95-53-4,
biological studies 95-57-8 95-68-1 95-76-1 95-80-7 95-82-9
96-37-7 98-07-7 98-54-4 98-82-8 99-65-0 100-00-5
100-21-0, biological studies 100-41-4, biological studies
100-42-5, biological studies 100-44-7, biological studies
100-51-6, biological studies 100-61-8, biological studies
100-66-3, biological studies 100-97-0, biological studies
101-53-1 101-84-8D, chloro derivs. 102-71-6, analysis 103-69-5
104-75-6 105-54-4 106-42-3, biological studies 106-43-4
106-44-5, biological studies 106-46-7 106-47-8, analysis
106-48-9 106-49-0, biological studies 106-99-0, analysis
107-05-1 107-06-2, biological studies 107-07-3, biological
studies 107-11-9 107-15-3, biological studies 107-19-7
107-21-1, biological studies 107-83-5 107-92-6, biological
studies 108-05-4, biological studies 108-38-3, biological
studies 108-39-4, biological studies 108-42-9 108-43-0
108-78-1, biological studies 108-88-3, biological studies
108-90-7, biological studies 108-91-8, biological studies
108-95-2, biological studies 109-86-4 109-89-7, biological
studies 110-54-3, biological studies 110-82-7, biological
studies 111-42-2, biological studies 111-46-6, biological
studies 111-65-9, biological studies 111-84-2 112-27-6
112-30-1 112-40-3 112-53-8 112-80-1, biological studies
112-95-8 115-32-2 115-77-5, analysis 117-18-0 117-81-7
118-74-1 119-07-3 119-36-8 120-32-1 120-36-5 120-80-9,
analysis 120-82-1 120-83-2 121-69-7, analysis 121-91-5,
biological studies 123-01-3 123-31-9, analysis 123-51-3
123-86-4 124-04-9, biological studies 124-04-9D, esters
124-09-4, biological studies 124-18-5 124-40-3, biological
studies 131-11-3 131-17-9 132-64-9D, chloro derivs. 139-13-9
141-43-5, biological studies 141-78-6, biological studies
142-82-5, biological studies 144-49-0 151-56-4, biological
studies 156-43-4 156-59-2 156-60-5 262-12-4D, chloro derivs.
309-00-2 527-20-8 540-84-1 542-75-6 544-76-3 554-00-7
576-24-9 **591-27-5** 629-50-5 629-59-4 629-62-9
629-78-7 629-92-5 629-97-0 1120-21-4 1321-67-1 1570-64-5
1582-09-8 1698-60-8 1825-21-4 1912-24-9 2631-68-7
2678-21-9 12789-03-6 25154-52-3 25264-93-1 25265-71-8
25322-68-3 25322-69-4 25339-56-4 25377-82-6 25377-83-7
25378-22-7 25551-13-7 26140-60-3 26140-60-3D, chloro derivs.
26761-40-0 26952-21-6 27043-34-1 27215-95-8 28761-27-5
28994-41-4 31394-54-4 31807-55-3 34464-38-5 34464-40-9
34464-43-2 38725-48-3 38725-49-4 61215-70-1 63597-41-1
70679-67-3 71030-52-9
RL: POL (Pollutant); OCCU (Occurrence)
(detn. of sources and retention of, in sewage sludges in
agricultural uses, health hazard in relation to)

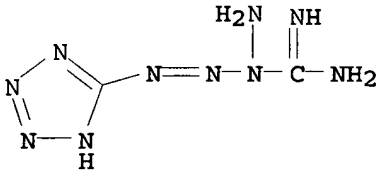
L66 ANSWER 9 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1979:577482 HCAPLUS
DOCUMENT NUMBER: 91:177482
TITLE: Spectrophotometric determination of tetrazene in primers and primer mixes by use of resorcinol
AUTHOR(S): Norwitz, George; Keliher, Peter N.
CORPORATE SOURCE: Chem. Dep., Villanova Univ., Villanova, PA, USA
SOURCE: Talanta (**1979**), 26(6), 451-4

CODEN: TLNTA2; ISSN: 0039-9140
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The spectrophotometric detn. of tetrazene [**31330-63-9**] involves treatment with resorcinol [**108-46-3**] and measurement of the intensity of the yellow **color** of the diazo **dye** formed. Pb styphnate and Ba(NO3)2 are first removed by extn. with aq. NH4OAc, and nitrocellulose and PETN are removed by extn. with Me2CO. The insol. residue is boiled with resorcinol, the soln. is filtered, and the absorbance at 400 nm is measured. Conditions for optimal **color** development are established and the nature of the reaction was examd. A primer was shown to contain 3.05-3.14% tetrazene by this method.

IT **31330-63-9**
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, in primers and primer mixes, resorcinol in spectrophotometric)

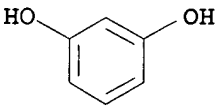
RN 31330-63-9 HCAPLUS
CN 3-Tetrazene-2-carboximidamide, 4-(1H-tetrazol-5-yl)-, monohydrate (9CI) (CA INDEX NAME)



● H_2O

IT **108-46-3**, uses and miscellaneous
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(in detn. of tetrazene in primers and primer mixes by spectrophotometry)

RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



CC 50-3 (Propellants and Explosives)
Section cross-reference(s): 80

IT **31330-63-9**
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, in primers and primer mixes, resorcinol in spectrophotometric)

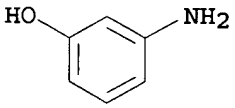
IT **108-46-3**, uses and miscellaneous
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(in detn. of tetrazene in primers and primer mixes by

spectrophotometry)

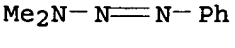
L66 ANSWER 10 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1976:516494 HCAPLUS
DOCUMENT NUMBER: 85:116494
TITLE: Urinary metabolites of 3,3-dimethyl-1-phenyltriazene
AUTHOR(S): Kolar, G. F.; Schlesiger, J.
CORPORATE SOURCE: Inst. Toxicol. Chemother., Ger. Cancer Res. Cent., Heidelberg, Fed. Rep. Ger.
SOURCE: Chemico-Biological Interactions (1976), 14(3-4), 301-11
CODEN: CBINA8; ISSN: 0009-2797
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Urinary metabolites excreted after a s.c. injection of 14C-labeled 3,3-dimethyl-1-phenyltriazene (I) [**7227-91-0**] to rats accounted for 82% of the applied radioactivity. Aniline [62-53-3] (1-2%), 2-hydroxyaniline [95-55-6](5-7%), 3-hydroxyaniline [**591-27-5**] (.apprx.1%), and 4-hydroxyaniline [123-30-8] (31-37%) were isolated from ethyl acetate exts. of acid-hydrolyzed urine. 4-Hydroxyaniline accounted for 56-61% of the applied dose. The excretion of metabolites contg. the intact triazene structure (0.9-1.1%) was demonstrated by cold acid cleavage of these compds., followed by coupling of the released arenediazonium cations with N-ethyl-1-naphthylamine-hydrochloride (EN) [36101-15-2]. The **colored** derivs. of these metabolites, 4-benzeneazo-N-ethyl-1-naphthylamine (BAEN) [60375-32-8] (0.6-0.7%), 4-(2-hydroxybenzeneazo)-N-ethyl-1-naphthylamine (2-HO-BAEN) [60375-33-9] (0.02%), and 4-(4-hydroxybenzeneazo)-N-ethyl-1-naphthylamine (4-HO-BAEN) [60375-34-0] (0.3-0.4%) were isolated. The identification of BAEN as the principal azo deriv. of the excreted triazene metabolites is in full agreement with the proposed in vivo activation of I to a carcinogenic methylating agent. The hydroxylation of the Me group at N-3 yields the corresponding aminol, some of which is covalently bonded to a water-sol. compd.

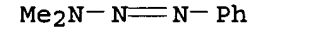
IT **591-27-5**
RL: BIOL (Biological study)
(as dimethylphenyltriazene metabolite)
RN 591-27-5 HCAPLUS
CN Phenol, 3-amino- (9CI) (CA INDEX NAME)



IT **7227-91-0**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(metab. of)
RN 7227-91-0 HCAPLUS
CN 1-Triazene, 3,3-dimethyl-1-phenyl- (9CI) (CA INDEX NAME)

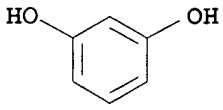


IT **58559-98-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 58559-98-1 HCAPLUS
CN 1-Triazene, 3,3-dimethyl-1-phenyl-, labeled with carbon-14 (9CI)
(CA INDEX NAME)

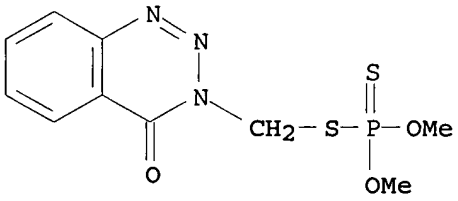


CC 1-2 (Pharmacodynamics)
Section cross-reference(s): 4
IT 62-53-3, biological studies 95-55-6 123-30-8 **591-27-5**
RL: BIOL (Biological study)
(as dimethylphenyltriazene metabolite)
IT **7227-91-0**
RL: BPR (Biological process); BSU (Biological study, unclassified);
BIOL (Biological study); PROC (Process)
(metab. of)
IT **58559-98-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L66 ANSWER 11 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1976:441999 HCAPLUS
DOCUMENT NUMBER: 85:41999
TITLE: Studies on azo-absorptiometrics. IX. Applications in pesticide analysis
AUTHOR(S): Gonzalez Garcia-Gutierrez, Alejo
CORPORATE SOURCE: Union Explos. Rio Tinto S. A., Madrid, Spain
SOURCE: Ion (Madrid) (**1975**), 35(412), 785-9, 809
CODEN: IONMAH; ISSN: 0375-9091
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
AB Methods are given for the detn. of pesticides, i.e. parathion [56-38-2], carbaryl [63-25-2], aminotriazole [61-82-5], azinphos-methyl [**86-50-0**], and α-substituted 2,4-dinitrophenol derivs., by diazo-coupling reactions with the coupling agents N-(1-naphthyl)ethylenediamine [551-09-7], resorcinol [**108-46-3**], and p-sulfanilic acid [121-57-3]. The **color** intensity of the resultant **dyes** was measured spectrophotometrically at 500-560 nm. Aminotriazole was nitrated, followed by coupling with N-(1-naphthyl)ethylenediamine or resorcinol, as usual. Parathion and azinphos methyl were first hydrolyzed and subsequently treated as above. Carbaryl was hydrolyzed and then treated with diazolized sulfanilic acid. 2,4-Dinitrophenol derivs. were reduced to the corresponding amines, then diazotized and reacted with the coupling agents.
IT **108-46-3**, uses and miscellaneous
RL: USES (Uses)
(coupling agent in pesticide detn. by diazo-coupling spectrophotometry)
RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



IT **86-50-0**
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by spectrophotometry following diazotation)
RN 86-50-0 HCAPLUS
CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



CC 5-1 (Agrochemicals)
IT **108-46-3**, uses and miscellaneous 121-57-3 551-09-7
RL: USES (Uses)
(coupling agent in pesticide detn. by diazo-coupling spectrophotometry)
IT **86-50-0**
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by spectrophotometry following diazotation)

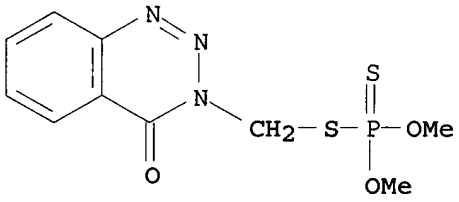
=> d l67 ibib abs hitstr hitind 1-31

L67 ANSWER 1 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:558355 HCAPLUS
DOCUMENT NUMBER: 135:284237
TITLE: Theoretical Descriptors for the Correlation of Aquatic Toxicity of Environmental Pollutants by Quantitative Structure-Toxicity Relationships
AUTHOR(S): Katritzky, Alan R.; Tatham, Douglas B.; Maran, Uko
CORPORATE SOURCE: Florida Institute of Heterocyclic Compounds Department of Chemistry, University of Florida, Gainesville, FL, 2611-7200, USA
SOURCE: Journal of Chemical Information and Computer Sciences (**2001**), 41(5), 1162-1176
CODEN: JCISD8; ISSN: 0095-2338
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Quant. structure-toxicity relationships were developed for the prediction of aq. toxicities for Poecilia reticulata (guppy) using the CODESSA treatment. A two-parameter correlation was found for class 1 toxins with R2 = 0.96, and a five-parameter correlation was found for class 2 toxins with R2 = 0.92. A five-parameter correlation for class 3 toxins had R2 = 0.85. The correlations for class 4 toxins were less satisfactory. All the descriptors utilized

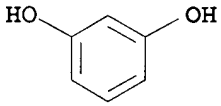
are calcd. solely from the structures of the mols., which makes it possible to predict unavailable or unknown toxins.

IT **86-50-0**, Azinphos-methyl **108-46-3**, 1,3-Dihydroxybenzene, biological studies
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(theor. descriptors for correlation of aquatic toxicity of environmental pollutants by quant. structure-toxicity relationships)

RN 86-50-0 HCAPLUS
CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



CC 4-3 (Toxicology)

IT 50-00-0, Methanal, biological studies 55-38-9, Fenthion 56-23-5, Tetrachloromethane, biological studies 58-89-9, Lindane 58-90-2, 2,3,4,6-Tetrachlorophenol 59-50-7, 4-Chloro-3-methylphenol 60-29-7, Diethyl ether, biological studies 60-57-1, Dieldrin 62-53-3, Aniline, biological studies 63-68-3, L-Methionine, biological studies 64-17-5, Ethanol, biological studies 66-25-1, Hexanal 67-56-1, Methanol, biological studies 67-63-0, 2-Propanol, biological studies 67-64-1, Acetone, biological studies 67-66-3, Chloroform, biological studies 67-72-1, Hexachloroethane 71-36-3, 1-Butanol, biological studies 71-43-2, Benzene, biological studies 71-55-6, 1,1,1-Trichloroethane 75-04-7, Ethylamine, biological studies 75-07-0, Ethanal, biological studies 75-09-2, Dichloromethane, biological studies 75-34-3, 1,1-Dichloroethane 75-56-9, Propylene oxide, biological studies 75-65-0, tert-Butanol, biological studies 75-97-8, 3,3-Dimethyl-2-butanone 76-01-7, Pentachloroethane 78-83-1, Isobutanol, biological studies 78-84-2, 2-Methylpropanal 78-87-5, 1,2-Dichloropropane 78-88-6, 2,3-Dichloropropene 78-93-3, 2-Butanone, biological studies 78-95-5, Chloroacetone 78-96-6, 1-Amino-2-propanol 79-00-5, 1,1,2-Trichloroethane 79-01-6, Trichloroethene, biological studies 79-06-1, Acrylamide, biological studies 79-34-5, 1,1,2,2-Tetrachloroethane 80-46-6, 4-tert-Pentylphenol 83-41-0, 2,3-Dimethylnitrobenzene 83-42-1, 2-Chloro-6-nitrotoluene 83-79-4, Rotenone **86-50-0**, Azinphos-methyl 87-61-6, 1,2,3-Trichlorobenzene 87-65-0, 2,6-Dichlorophenol 87-68-3, Hexachlorobutadiene 87-86-5,

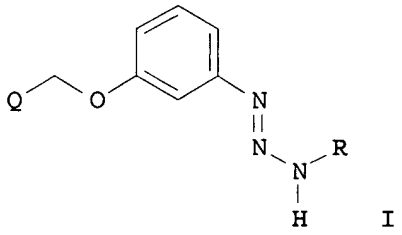
Pentachlorophenol 88-04-0, 4-Chloro-3,5-dimethylphenol 88-06-2, 2,4,6-Trichlorophenol 88-72-2, 2-Nitrotoluene 88-73-3, 2-Chloronitrobenzene 88-74-4, 2-Nitroaniline 88-85-7, 2-sec-Butyl-4,6-dinitrophenol 89-59-8, 4-Chloro-2-nitrotoluene 89-61-2, 2,5-Dichloronitrobenzene 90-15-3, 1-Naphthalenol 90-43-7, 2-Phenylphenol 91-22-5, Quinoline, biological studies 94-99-5, 2,4,α-Trichlorotoluene 95-47-6, biological studies 95-48-7, 2-Methylphenol, biological studies 95-50-1, 1,2-Dichlorobenzene 95-51-2, 2-Chloroaniline 95-53-4, 2-Methylaniline, biological studies 95-57-8, 2-Chlorophenol 95-65-8, 3,4-Dimethylphenol 95-73-8, 2,4-Dichlorotoluene 95-75-0, 3,4-Dichlorotoluene 95-76-1, 3,4-Dichloroaniline 95-82-9, 2,5-Dichloroaniline 95-94-3, 1,2,4,5-Tetrachlorobenzene 95-95-4, 2,4,5-Trichlorophenol 96-09-3, Styrene oxide 96-18-4, 1,2,3-Trichloropropane 96-22-0, 3-Pentanone 97-00-7, 1-Chloro-2,4-dinitrobenzene 97-77-8, Disulfiram 97-96-1, 2-Ethylbutanal 98-01-1, 2-Furaldehyde, biological studies 98-54-4, 4-tert-Butylphenol 98-86-2, Acetophenone, biological studies 98-95-3, Nitrobenzene, biological studies 99-08-1, 3-Nitrotoluene 99-09-2, 3-Nitroaniline 99-51-4 99-65-0, 1,3-Dinitrobenzene 99-99-0, 4-Nitrotoluene 100-00-5, 4-Chloronitrobenzene 100-01-6, 4-Nitroaniline, biological studies 100-02-7, 4-Nitrophenol, biological studies 100-44-7, Benzyl chloride, biological studies 100-46-9, Benzylamine, biological studies 100-50-5, 3-Cyclohexene-1-carboxaldehyde 100-52-7, Benzaldehyde, biological studies 101-84-8, Diphenyl ether 104-13-2, 4-Butylaniline 104-40-5, 4-Nonylphenol 105-67-9, 2,4-Dimethylphenol 106-40-1, 4-Bromoaniline 106-42-3, biological studies 106-43-4, 4-Chlorotoluene 106-44-5, 4-Methylphenol, biological studies 106-46-7, 1,4-Dichlorobenzene 106-47-8, 4-Chloroaniline, biological studies 106-48-9, 4-Chlorophenol 106-49-0, 4-Methylaniline, biological studies 106-88-7, 1,2-Epoxybutane 106-89-8, Epichlorohydrin, biological studies 107-05-1, Allyl chloride 107-06-2, 1,2-Dichloroethane, biological studies 107-10-8, Propylamine, biological studies 107-18-6, Allyl alcohol, biological studies 107-21-1, 1,2-Ethanediol, biological studies 107-41-5, 2-Methyl-2,4-pentanediol 107-45-9, tert-Octylamine 108-10-1, 4-Methyl-2-pentanone 108-20-3, Diisopropyl ether 108-38-3, biological studies 108-39-4, 3-Methylphenol, biological studies 108-41-8, 3-Chlorotoluene 108-42-9, 3-Chloroaniline 108-43-0, 3-Chlorophenol 108-44-1, 3-Methylaniline, biological studies **108-46-3**, 1,3-Dihydroxybenzene, biological studies 108-70-3, 1,3,5-Trichlorobenzene 108-88-3, Toluene, biological studies 108-90-7, Chlorobenzene, biological studies 108-93-0, Cyclohexanol, biological studies 108-94-1, Cyclohexanone, biological studies 108-95-2, Phenol, biological studies 109-59-1, 2-Isopropoxyethanol 109-69-3, 1-Chlorobutane 109-73-9, Butylamine, biological studies 109-85-3, 2-Methoxyethylamine 109-86-4, 2-Methoxyethanol 109-99-9, Tetrahydrofuran, biological studies 110-00-9, Furan 110-58-7, Amylamine 110-62-3, Pentanal 110-80-5, 2-Ethoxyethanol 110-93-0, 6-Methyl-5-hepten-2-one 111-13-7, 2-Octanone 111-26-2, Hexylamine 111-27-3, 1-Hexanol, biological studies 111-44-4, 2,2'-Dichlorodiethyl ether 111-46-6, Diethyleneglycol, biological studies 111-68-2, Heptylamine 111-71-7, Heptanal 111-76-2, 2-Butoxyethanol 111-86-4, Octylamine 111-87-5, 1-Octanol, biological studies 111-90-0, 2-(2-Ethoxyethoxy)ethanol 112-20-9, Nonylamine 112-27-6, Triethyleneglycol 112-30-1, 1-Decanol 112-31-2, Decanal 112-34-5, Butyldigol 112-42-5, 1-Undecanol 112-53-8,

1-Dodecanol 112-56-1, Lethane 115-20-8, 2,2,2-Trichloroethanol 118-79-6, 2,4,6-Tribromophenol 119-34-6, 4-Amino-2-nitrophenol 119-61-9, Benzophenone, biological studies 120-82-1, 1,2,4-Trichlorobenzene 120-83-2, 2,4-Dichlorophenol 121-69-7, N,N-Dimethylaniline, biological studies 121-73-3, 3-Chloronitrobenzene 121-87-9, 2-Chloro-4-nitroaniline 122-14-5, Fenitrothion 122-99-6, 2-Phenoxyethanol 123-07-9, 4-Ethylphenol 123-38-6, Propanal, biological studies 123-72-8, Butanal 124-13-0, Octanal 124-22-1, Dodecylamine 127-18-4, Tetrachloroethene, biological studies 136-77-6, 4-Hexylresorcinol 140-88-5, Ethyl acrylate 141-43-5, 2-Aminoethanol, biological studies 142-28-9, 1,3-Dichloropropane 142-96-1, Dibutyl ether 143-08-8, 1-Nonanol 148-24-3, 8-Hydroxyquinoline, biological studies 150-19-6, 3-Methoxyphenol 150-76-5, 4-Methoxyphenol 150-78-7, 1,4-Dimethoxybenzene 298-00-0, Methylparathion 299-84-3, Ronnel 329-71-5, 2,5-Dinitrophenol 393-39-5, α,α,α,4-Tetrafluoro-2-methylaniline 500-28-7, Chlorothion 502-56-7, 5-Nonanone 541-73-1, 1,3-Dichlorobenzene 542-75-6, 1,3-Dichloropropene 552-41-0 554-00-7, 2,4-Dichloroaniline 554-84-7, 3-Nitrophenol 556-52-5, Glycidol 563-52-0, 3-Chloro-1-butene 563-80-4, 3-Methyl-2-butanone 576-26-1, 2,6-Dimethylphenol 578-54-1, 2-Ethylaniline 583-78-8, 2,5-Dichlorophenol 584-02-1, 3-Pentanol 587-02-0, 3-Ethylaniline 589-16-2, 4-Ethylaniline 590-86-3, 3-Methylbutanal 591-35-5, 3,5-Dichlorophenol 591-97-9, 1-Chloro-2-butene 598-74-3, 1,2-Dimethylpropylamine 608-93-5, Pentachlorobenzene 609-19-8, 3,4,5-Trichlorophenol 611-06-3, 2,4-Dichloronitrobenzene 616-86-4, 4-Ethoxy-2-nitroaniline 618-62-2, 3,5-Dichloronitrobenzene 626-43-7, 3,5-Dichloroaniline 634-66-2, 1,2,3,4-Tetrachlorobenzene 634-67-3, 2,3,4-Trichloroaniline 634-83-3, 2,3,4,5-Tetrachloroaniline 634-90-2, 1,2,3,5-Tetrachlorobenzene 636-30-6, 2,4,5-Trichloroaniline 640-19-7, Fluoroacetamide 645-56-7, 4-Propylphenol 693-16-3, 1-Methylheptylamine 693-54-9, 2-Decanone 693-65-2, Dipentyl ether 732-11-6, Phosmet 764-41-0, 1,4-Dichloro-2-butene 768-94-5, 1-Adamantanamine 771-60-8, Pentafluoroaniline 831-82-3, 4-Phenoxyphenol 933-75-5, 2,3,6-Trichlorophenol 933-78-8, 2,3,5-Trichlorophenol 935-95-5, 2,3,5,6-Tetrachlorophenol 950-37-8, Methidathion
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(theor. descriptors for correlation of aquatic toxicity of environmental pollutants by quant. structure-toxicity relationships)

REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L67 ANSWER 2 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:745386 HCAPLUS
DOCUMENT NUMBER: 134:71122
TITLE: Solid-phase synthesis of urea and amide libraries using the T2 triazene linker
AUTHOR(S): Braese, Stefan; Dahmen, Stefan; Pfefferkorn, Marc
CORPORATE SOURCE: Institut fuer Organische Chemie, RWTH Aachen, Aachen, 52074, Germany
SOURCE: Journal of Combinatorial Chemistry (2000), 2(6), 710-715
CODEN: JCCHFF; ISSN: 1520-4766

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:71122
GI

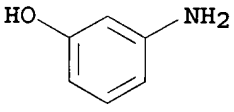


I

AB Starting from Merrifield resin, primary amines were immobilized in two steps by triazene linkage (T2-linker) to give triazene resins I [Q = Merrifield resin; R = allyl, benzyl, HOCH2CH2CH2, (S)-PhCHMe, cyclopropyl, (R)-PhCH2CH(NH2)CO2Me]. Reaction I with isocyanates gave resin-bound ureas and acylation of I by acid chlorides or acid anhydrides gave amides bound to the solid support via the nitrogen atom, therefore representing a novel backbone amide linker. Cleavage from the resin was conducted using dil. trimethylsilyl chloride or trifluoroacetic acid, resp., to yield ureas and amines/amides in a library format in high purity and good overall yields. Manual synthesis using this procedure gave seventeen ureas and six mono-alkylated ureas that included dihydroxylation and ozonolysis/Wittig olefination reaction products, and an automated synthesis yielded fifteen ureas and fifteen amides. The synthesis of a small library (4 + 4 member) was successfully conducted on a Bohdan-Neptune synthesizer.

IT **591-27-5**, 3-Aminophenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(solid-phase synthesis of urea and amide libraries by reaction of T2 triazene linker immobilized primary amines with isocyanates and acid chlorides)

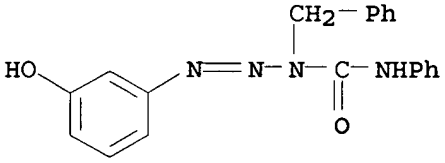
RN 591-27-5 HCAPLUS
CN Phenol, 3-amino- (9CI) (CA INDEX NAME)



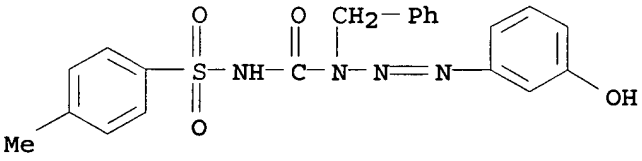
IT **316180-59-3DP**, resin-bound **316180-60-6DP**, resin-bound **316180-61-7DP**, resin-bound **316180-62-8DP**, resin-bound **316180-63-9DP**, resin-bound **316180-64-0DP**, resin-bound **316180-65-1DP**, resin-bound **316180-66-2DP**, resin-bound **316180-67-3DP**, resin-bound **316180-68-4DP**, resin-bound **316180-69-5DP**, resin-bound **316180-70-8DP**, resin-bound **316180-71-9DP**, resin-bound **316180-72-0DP**,

resin-bound **316180-73-1DP**, resin-bound
316180-74-2DP, resin-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(solid-phase synthesis of urea and amide libraries by reaction of T2 triazene linker immobilized primary amines with isocyanates and acid chlorides)

RN 316180-59-3 HCAPLUS
CN 2-Triazene-1-carboxamide, 3-(3-hydroxyphenyl)-N-phenyl-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

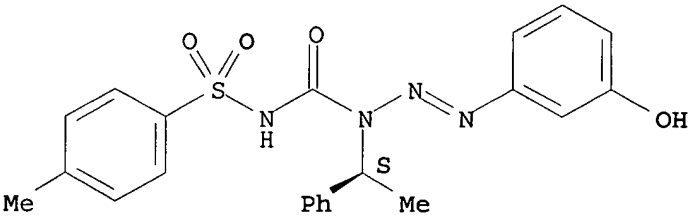


RN 316180-60-6 HCAPLUS
CN 2-Triazene-1-carboxamide, 3-(3-hydroxyphenyl)-N-[(4-methylphenyl)sulfonyl]-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

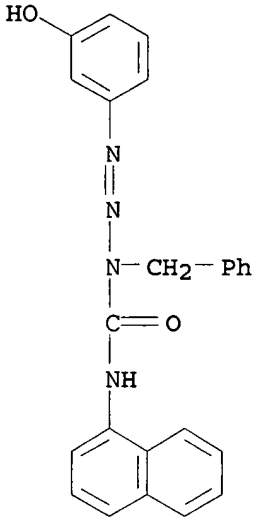


RN 316180-61-7 HCAPLUS
CN 2-Triazene-1-carboxamide, 3-(3-hydroxyphenyl)-N-[(4-methylphenyl)sulfonyl]-1-[(1S)-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

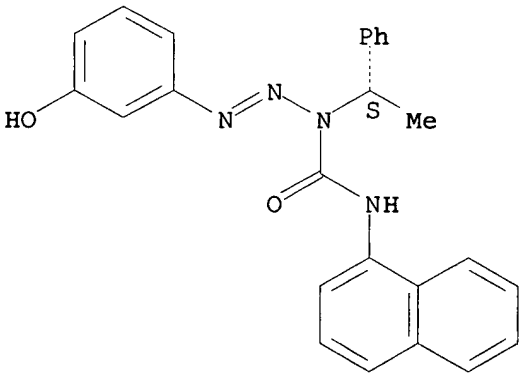


RN 316180-62-8 HCAPLUS
CN 2-Triazene-1-carboxamide, 3-(3-hydroxyphenyl)-N-1-naphthalenyl-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

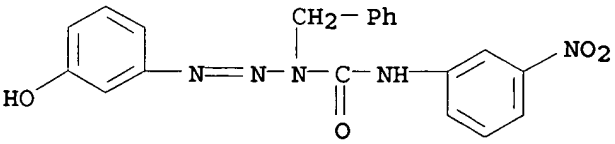


RN 316180-63-9 HCAPLUS
CN 2-Triazene-1-carboxamide, 3-(3-hydroxyphenyl)-N-1-naphthalenyl-1-[(1S)-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

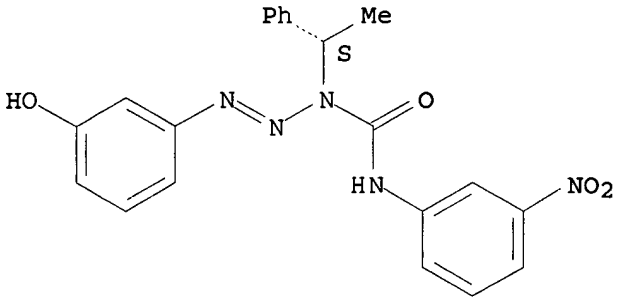


RN 316180-64-0 HCAPLUS
CN 2-Triazene-1-carboxamide, 3-(3-hydroxyphenyl)-N-(3-nitrophenyl)-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

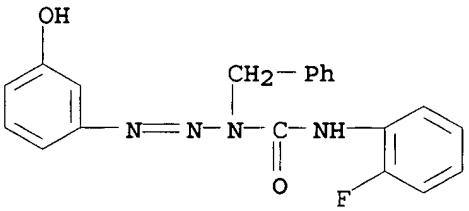


RN 316180-65-1 HCAPLUS
CN 2-Triazene-1-carboxamide, 3-(3-hydroxyphenyl)-N-(3-nitrophenyl)-1-[(1S)-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

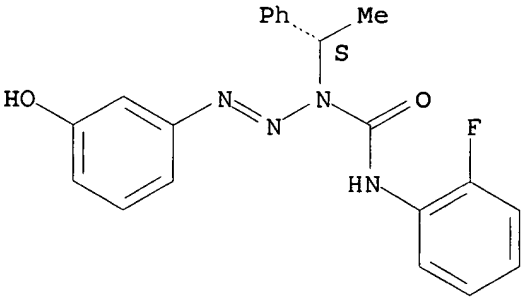


RN 316180-66-2 HCAPLUS
CN 2-Triazene-1-carboxamide, N-(2-fluorophenyl)-3-(3-hydroxyphenyl)-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

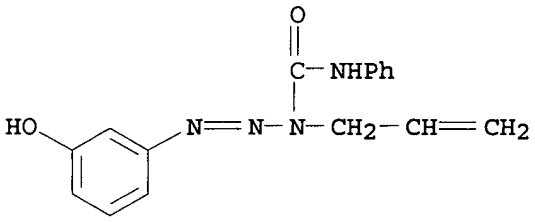


RN 316180-67-3 HCAPLUS
CN 2-Triazene-1-carboxamide, N-(2-fluorophenyl)-3-(3-hydroxyphenyl)-1-[(1S)-1-phenylethyl]- (9CI) (CA INDEX NAME)

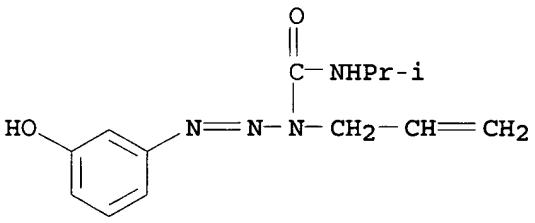
Absolute stereochemistry.
Double bond geometry unknown.



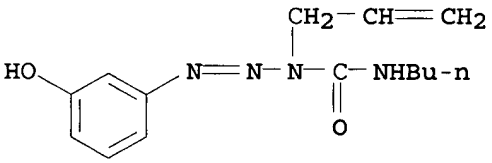
RN 316180-68-4 HCAPLUS
CN 2-Triazene-1-carboxamide, 3-(3-hydroxyphenyl)-N-phenyl-1-(2-propenyl)- (9CI) (CA INDEX NAME)



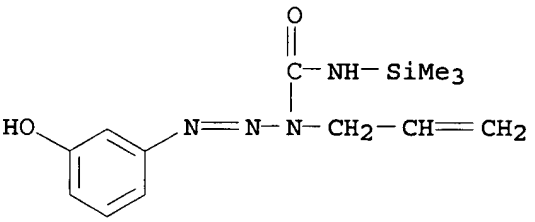
RN 316180-69-5 HCAPLUS
CN 2-Triazene-1-carboxamide, 3-(3-hydroxyphenyl)-N-(1-methylethyl)-1-(2-propenyl)- (9CI) (CA INDEX NAME)



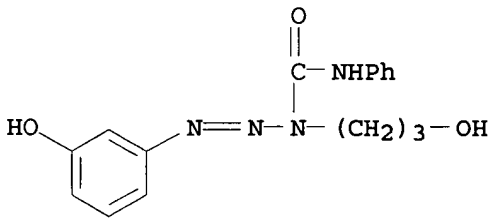
RN 316180-70-8 HCAPLUS
CN 2-Triazene-1-carboxamide, N-butyl-3-(3-hydroxyphenyl)-1-(2-propenyl)- (9CI) (CA INDEX NAME)



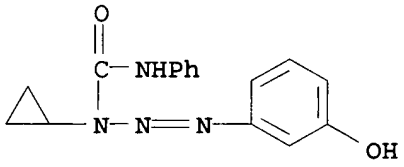
RN 316180-71-9 HCAPLUS
CN 2-Triazene-1-carboxamide, 3-(3-hydroxyphenyl)-1-(2-propenyl)-N-(trimethylsilyl)- (9CI) (CA INDEX NAME)



RN 316180-72-0 HCAPLUS
CN 2-Triazene-1-carboxamide, 3-(3-hydroxyphenyl)-1-(3-hydroxypropyl)-N-phenyl- (9CI) (CA INDEX NAME)

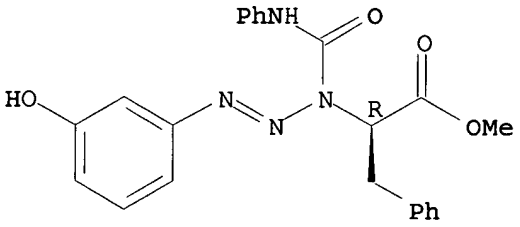


RN 316180-73-1 HCAPLUS
CN 2-Triazene-1-carboxamide, 1-cyclopropyl-3-(3-hydroxyphenyl)-N-phenyl- (9CI) (CA INDEX NAME)



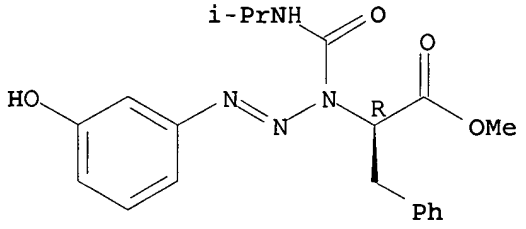
RN 316180-74-2 HCAPLUS
CN Benzenepropanoic acid, α-[3-(3-hydroxyphenyl)-1-[(phenylamino)carbonyl]-2-triazenyl]-, methyl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



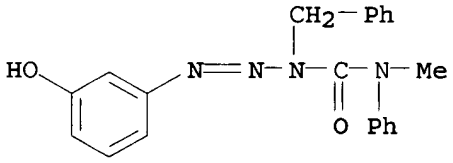
IT **316180-75-3DP**, resin-bound
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid-phase synthesis of urea and amide libraries by reaction of T2 triazene linker immobilized primary amines with isocyanates and acid chlorides)
RN 316180-75-3 HCAPLUS
CN Benzenepropanoic acid, α-[3-(3-hydroxyphenyl)-1-[[(1-methylethyl)amino]carbonyl]-2-triazenyl]-, methyl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

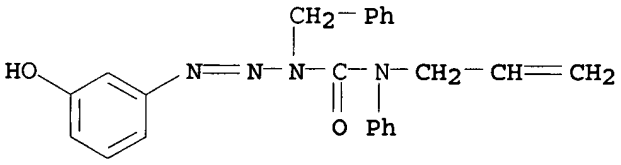


IT **316180-76-4DP**, resin-bound **316180-77-5DP**, resin-bound **316180-78-6DP**, resin-bound **316180-79-7DP**, resin-bound **316180-80-0DP**, resin-bound **316180-81-1DP**, resin-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(solid-phase synthesis of urea libraries by reaction of T2 triazene linker immobilized primary amines with isocyanates and subsequent alkylation)

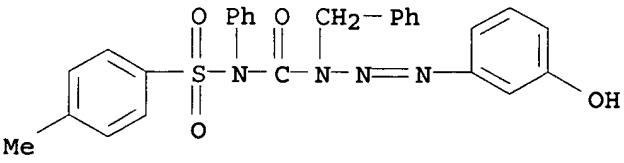
RN 316180-76-4 HCAPLUS
CN 2-Triazene-1-carboxamide, 3-(3-hydroxyphenyl)-N-methyl-N-phenyl-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



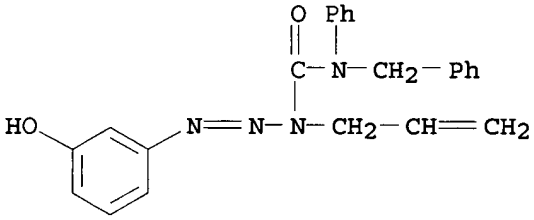
RN 316180-77-5 HCAPLUS
CN 2-Triazene-1-carboxamide, 3-(3-hydroxyphenyl)-N-phenyl-1-(phenylmethyl)-N-2-propenyl- (9CI) (CA INDEX NAME)



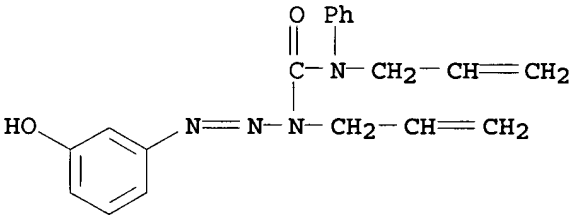
RN 316180-78-6 HCAPLUS
CN 2-Triazene-1-carboxamide, 3-(3-hydroxyphenyl)-N-[(4-methylphenyl)sulfonyl]-N-phenyl-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



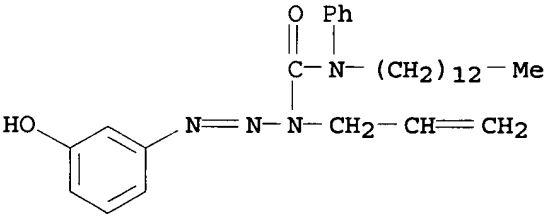
RN 316180-79-7 HCAPLUS
CN 2-Triazene-1-carboxamide, 3-(3-hydroxyphenyl)-N-phenyl-N-(phenylmethyl)-1-(2-propenyl)- (9CI) (CA INDEX NAME)



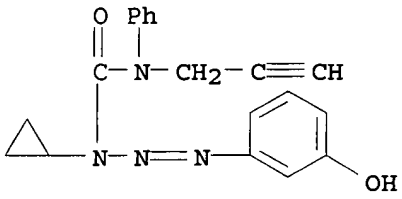
RN 316180-80-0 HCAPLUS
CN 2-Triazene-1-carboxamide, 3-(3-hydroxyphenyl)-N-phenyl-N,1-di-2-propenyl- (9CI) (CA INDEX NAME)



RN 316180-81-1 HCAPLUS
CN 2-Triazene-1-carboxamide, 3-(3-hydroxyphenyl)-N-phenyl-1-(2-propenyl)-N-tridecyl- (9CI) (CA INDEX NAME)

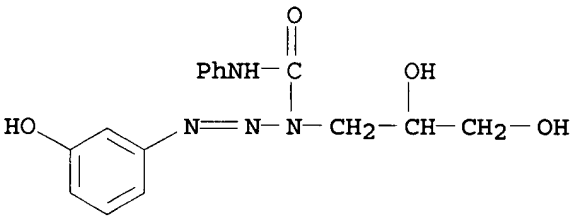


IT **316180-82-2DP**, resin-bound
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid-phase synthesis of urea libraries by reaction of T2 triazene linker immobilized primary amines with isocyanates and subsequent alkylation)
RN 316180-82-2 HCAPLUS
CN 2-Triazene-1-carboxamide, 1-cyclopropyl-3-(3-hydroxyphenyl)-N-phenyl-N-2-propynyl- (9CI) (CA INDEX NAME)

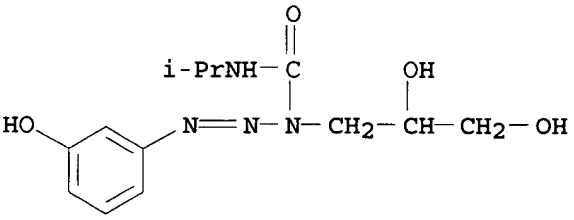


IT **316180-83-3DP**, resin-bound **316180-84-4DP**, resin-bound **316180-85-5DP**, resin-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(solid-phase synthesis of urea libraries by reaction of T2 triazene linker immobilized primary amines with isocyanates and subsequent hydroxylation and ozonolysis/olefination reactions)

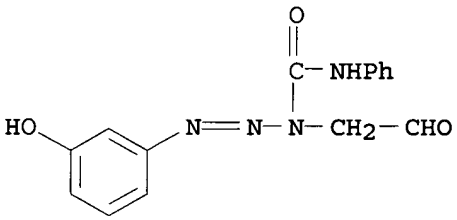
RN 316180-83-3 HCAPLUS
CN 2-Triazene-1-carboxamide, 1-(2,3-dihydroxypropyl)-3-(3-hydroxyphenyl)-N-phenyl- (9CI) (CA INDEX NAME)



RN 316180-84-4 HCAPLUS
CN 2-Triazene-1-carboxamide, 1-(2,3-dihydroxypropyl)-3-(3-hydroxyphenyl)-N-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 316180-85-5 HCAPLUS
CN 2-Triazene-1-carboxamide, 3-(3-hydroxyphenyl)-1-(2-oxoethyl)-N-phenyl- (9CI) (CA INDEX NAME)



CC 21-2 (General Organic Chemistry)

IT 75-36-5, Acetyl chloride 79-04-9, Chloroacetyl chloride 86-84-0, 1-Naphthyl isocyanate 100-46-9, Benzylamine, reactions 103-71-9, Phenyl isocyanate, reactions 107-11-9, Allyl amine 111-36-4, Butyl isocyanate 122-04-3, 4-Nitrobenzoyl chloride 156-87-6, 3-Amino-1-propanol **591-27-5**, 3-Aminophenol 765-30-0, Cyclopropylamine 1118-02-1, Trimethylsilyl isocyanate 1795-48-8, Isopropyl isocyanate 2627-86-3, (S)-1-Phenylethylamine 3320-87-4, 3-Nitrophenyl isocyanate 4083-64-1 16744-98-2, 2-Fluorophenyl isocyanate 21685-51-8, D-Phenylalanine methyl ester 22118-09-8, Bromoacetyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(solid-phase synthesis of urea and amide libraries by reaction of T2 triazene linker immobilized primary amines with isocyanates and acid chlorides)

IT 264230-85-5DP, resin-bound 316180-54-8DP, resin-bound 316180-55-9DP, resin-bound 316180-56-0DP, resin-bound 316180-57-1DP, resin-bound 316180-58-2DP, resin-bound **316180-59-3DP**, resin-bound **316180-60-6DP**, resin-bound **316180-61-7DP**, resin-bound **316180-62-8DP**, resin-bound **316180-63-9DP**, resin-bound **316180-64-0DP**, resin-bound **316180-65-1DP**, resin-bound **316180-66-2DP**, resin-bound **316180-67-3DP**, resin-bound **316180-68-4DP**, resin-bound **316180-69-5DP**, resin-bound **316180-70-8DP**, resin-bound **316180-71-9DP**, resin-bound **316180-72-0DP**, resin-bound **316180-73-1DP**, resin-bound **316180-74-2DP**, resin-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(solid-phase synthesis of urea and amide libraries by reaction of T2 triazene linker immobilized primary amines with isocyanates and acid chlorides)

IT 588-46-5P, N-Benzylacetamide 692-33-1P, N-Allylacetamide 1467-21-6P, N-Benzyl-N'-phenylurea 1801-72-5P, 1,3-Diallylurea 1987-58-2P 2564-06-9P 2585-26-4P 2835-30-5P 2945-03-1P 4974-07-6P 13140-86-8P 13141-77-0P 13256-79-6P 13269-97-1P, N-Allyl-2-chloroacetamide 19035-02-0P 19144-86-6P 33251-70-6P 36293-01-3P 68423-09-6P 88229-26-9P 89607-27-2P 101112-21-4P 101401-80-3P 101570-38-1P 109905-77-3P 126265-30-3P 132104-27-9P 137036-01-2P 138088-48-9P 193967-71-4P 194788-50-6P 194788-53-9P 194801-91-7P **316180-75-3DP**, resin-bound 316180-86-6P 316180-87-7P 316180-88-8P 316180-89-9P 316180-90-2P 316180-91-3P 316180-92-4P 316180-93-5P 316180-94-6P 316180-95-7P 316180-96-8P 316180-97-9P 316180-98-0P 316180-99-1P 316181-00-7P 316181-01-8P 316181-02-9P
RL: SPN (Synthetic preparation); PREP (Preparation)

(solid-phase synthesis of urea and amide libraries by reaction of T2 triazene linker immobilized primary amines with isocyanates and acid chlorides)

IT **316180-76-4DP**, resin-bound **316180-77-5DP**, resin-bound **316180-78-6DP**, resin-bound **316180-79-7DP**, resin-bound **316180-80-0DP**, resin-bound **316180-81-1DP**, resin-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(solid-phase synthesis of urea libraries by reaction of T2 triazene linker immobilized primary amines with isocyanates and subsequent alkylation)

IT **316180-82-2DP**, resin-bound
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid-phase synthesis of urea libraries by reaction of T2 triazene linker immobilized primary amines with isocyanates and subsequent alkylation)

IT **316180-83-3DP**, resin-bound **316180-84-4DP**, resin-bound **316180-85-5DP**, resin-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(solid-phase synthesis of urea libraries by reaction of T2 triazene linker immobilized primary amines with isocyanates and subsequent hydroxylation and ozonolysis/olefination reactions)

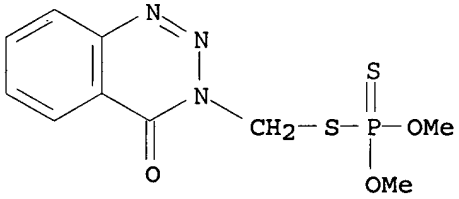
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L67 ANSWER 3 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:473354 HCAPLUS
DOCUMENT NUMBER: 134:111334
TITLE: A study on the screening of toxic materials by HPTLC and GC/MS
AUTHOR(S): Park, Sung-Woo; Jang, Seong-Gil; Park, Ou-Sin; Lee, Jin-Hoon; Lee, Sang-Ki; You, Jae-Hoon; Kim, Dong-Hwan; Jin, Kwang-Ho; Kim, Ki-Wook; Kim, Yu-Na; Lho, Dong-Seok
CORPORATE SOURCE: National Institute of Scientific Investigation, Seoul, 158-097, S. Korea
SOURCE: Analytical Science & Technology (**2000**), 13(1), 108-120
CODEN: ASCTET; ISSN: 1225-0163
PUBLISHER: Korean Society of Analytical Sciences
DOCUMENT TYPE: Journal
LANGUAGE: Korean

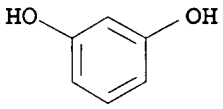
AB To perform an effective screening for toxic materials of forensic interest detected in high profile criminal cases in biol. and environmental samples, the authors tried to construct a searchable computerized database using HPTLC (high-performance thin-layer chromatog.) and GC/MS. Retardation factor (R4) values and UV spectral data of HPTLC were investigated for 160 pesticides, 34 chems., and 39 explosives of std. grade. The data were compiled in a library. The authors also analyzed 112 pesticides, 31 chems., and 17 explosives and 57 volatile org. compds. (VOCs) by GC/MS. The data for RT and characteristic mass ions were also compiled in a library.

IT **86-50-0**, Azinphos-methyl **108-46-3**, Resorcinol, analysis
RL: ANT (Analyte); ANST (Analytical study)
(screening of toxic materials by high-performance TLC and GC/MS)

RN 86-50-0 HCAPLUS
CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



CC 4-2 (Toxicology)
IT 50-29-3, DDT, analysis 51-03-6, Piperonyl butoxide 51-28-5, 2,4-Dinitrophenol, analysis 55-38-9, Fenthion 55-63-0, Nitroglycerine 56-23-5, Carbon tetrachloride, analysis 56-38-2, Parathion 56-72-4, Coumaphos 58-89-9, BHC 59-88-1, Phenylhydrazine hydrochloride 60-51-5, Dimethoate 62-53-3, Aniline, analysis 62-73-7, Dichlorvos 63-25-2, Carbaryl 65-85-0, Benzoic acid, analysis 67-66-3, Chloroform, analysis 71-43-2, Benzene, analysis 71-55-6, 1,1,1-Trichloroethane 72-20-8, Endrin 72-43-5, Methoxychlor 72-54-8, TDE 72-55-9, DDE, analysis 72-56-0, Perthane 74-83-9, Bromomethane, analysis 74-87-3, Chloromethane, analysis 74-97-5, Bromochloromethane 75-00-3, Chloroethane 75-09-2, Methylene chloride, analysis 75-25-2, Bromoform 75-27-4, Bromodichloromethane 75-34-3, 1,1-Dichloroethane 75-35-4, 1,1-Dichloroethylene, analysis 75-69-4, Trichlorofluoromethane 76-44-8, Heptachlor 78-11-5, Tetranitropentaerythritol 78-87-5, 1,2-Dichloropropane 79-00-5, 1,1,2-Trichloroethane 79-01-6, Trichloroethylene, analysis 79-34-5, 1,1,2,2-Tetrachloroethane 81-81-2, Warfarin 82-68-8, Quintozene 83-26-1, Pindone 84-66-2, Diethylphthalate 84-74-2, Butyl phthalate **86-50-0**, Azinphos-methyl 86-57-7, 1-Nitronaphthalene 87-41-2, Phthalide 87-51-4, 1H-Indole-3-acetic acid, analysis 87-61-6, 1,2,3-Trichlorobenzene 87-68-3, Hexachlorobutadiene 88-06-2, 2,4,6-Trichlorophenol 88-85-7, Dinoseb 88-89-1, Picric acid 91-20-3, Naphthalene, analysis 91-64-5, Coumarin 93-65-2, Mecoprop 93-72-1, Silvex 93-76-5, 2,4,5-T 94-75-7, 2,4-D, analysis 94-82-6, 2,4-DB 95-06-7, Sulfallate 95-47-6, o-Xylene, analysis 95-49-8, 2-Chlorotoluene 95-50-1, o-Dichlorobenzene 95-53-4, o-Toluidine, analysis 95-63-6, 1,2,4-Trimethylbenzene 95-77-2, 3,4-Dichlorophenol 95-88-5, 4-Chlororesorcinol 95-95-4, 2,4,5-Trichlorophenol 96-12-8, Nemagon 96-18-4, 1,2,3-Trichloropropane 97-00-7, Dinitrochlorobenzene 98-06-6, tert-Butylbenzene 98-82-8, Isopropylbenzene 98-95-3, Nitrobenzene, analysis 99-30-9, Dicloran 99-35-4, 1,3,5-Trinitrobenzene 99-65-0, 1,3-Dinitrobenzene 99-87-6,

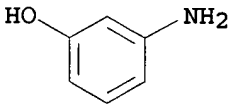
p-Isopropyltoluene 100-02-7, p-Nitrophenol, analysis 100-41-4, Ethylbenzene, analysis 100-42-5, Styrene, analysis 101-05-3, Anilazine 101-21-3, Chlorpropham 103-65-1, n-Propylbenzene 104-51-8, n-Butylbenzene 106-42-3, p-Xylene, analysis 106-46-7, 1,4-Dichlorobenzene 106-93-4, 1,2-Dibromoethane 107-06-2, 1,2-Dichloroethane, analysis 108-38-3, m-Xylene, analysis 108-39-4, m-Cresol, analysis 108-45-2, m-Phenylenediamine, analysis **108-46-3**, Resorcinol, analysis 108-67-8, 1,3,5-Trimethylbenzene, analysis 108-86-1, Bromobenzene, analysis 108-88-3, Toluene, analysis 108-90-7, Chlorobenzene, analysis 108-95-2, Phenol, analysis 114-26-1, Propoxur 115-29-7, Endosulfan 115-32-2, Dicofol 115-90-2, Fensulfothion 116-29-0, Tetradifon 117-81-7, Dioctylphthalate 118-75-2, Chloranil, analysis 118-96-7, TNT 119-26-6 119-75-5, 2-Nitrodiphenylamine 120-12-7, Anthracene, analysis 120-80-9, Catechol, analysis 120-82-1, 1,2,4-Trichlorobenzene 120-83-2, 2,4-Dichlorophenol 121-14-2, 2,4-Dinitrotoluene 121-82-4, Trimethylenetrinitramine 122-14-5, Fenitrothion 122-34-9, Simazine 122-39-4, Diphenylamine, analysis 123-07-9, 4-Ethylphenol 123-31-9, Hydroquinone, analysis 123-33-1 124-48-1, Dibromochloromethane 127-18-4, Tetrachloroethylene, analysis 128-37-0, BHT, analysis 131-11-3, Dimethylphthalate 133-06-2, Captan 133-07-3, Folpet 135-19-3, β-Naphthol, analysis 135-98-8, sec-Butylbenzene 139-40-2, Propazin 142-28-9, 1,3-Dichloropropane 148-24-3, 8-Quinolinol, analysis 148-79-8, Thiabendazole 150-68-5, Monuron 156-59-2, cis-1,2-Dichloroethylene 156-60-5, trans-1,2-Dichloroethylene 298-00-0, Methyl parathion 298-02-2, Phorate 298-04-4, Disulfoton 299-84-3, Fenchlorphos 299-86-5, Crufomate 301-12-2, Oxydemeton methyl 309-00-2, Aldrin 314-40-9, Bromacil 330-54-1, Diuron 330-55-2, Linuron 333-41-5, Diazinon 470-90-6, Chlorfenvinphos 479-45-8, Tetryl 495-69-2, Hippuric acid 510-15-6, Chlorobenzilate 528-29-0, 1,2-Dinitrobenzene 538-62-5, Diphenylcarbazone 541-73-1, 1,3-Dichlorobenzene 563-12-2, Ethion 563-58-6, 1,1-Dichloropropylene 573-56-8, 2,6-Dinitrophenol 576-24-9, 2,3-Dichlorophenol 583-78-8, 2,5-Dichlorophenol 584-79-2, Allethrin 594-20-7, 2,2-Dichloropropane 602-38-0, 1,8-Dinitronaphthalene 606-20-2, 2,6-Dinitrotoluene 610-39-9, 3,4-Dinitrotoluene 628-96-6, Nitroglycol 630-20-6, 1,1,1,2-Tetrachloroethane 709-98-8, Propanil 732-11-6, Phosmet 786-19-6, Carbophenothion 944-22-9, Fonofos 950-37-8, Methidathion 1024-57-3, Epoxyheptachlor 1085-98-9, Dichlofluanide 1113-02-6, Omethoate 1129-41-5, Metolcarb 1194-65-6, Dichlobenil 1214-39-7 1563-66-2, Carbofuran 1582-09-8, Trifluralin 1861-32-1, Chlorthal-methyl 1897-45-6, Chlorothalonil 1912-24-9, Atrazine 1918-00-9, Dicamba 1918-11-2, Terbucarb 1918-16-7, Propachlor 1928-37-6, 2,4,5-T Methyl ester 2078-24-2 2104-64-5, EPN 2212-67-1, Molinate 2274-67-1, Dimethylvinphos 2275-23-2, Vamidothion 2303-17-5, Tri-allate 2310-17-0, Phosalone 2312-35-8 2425-06-1, Captafol 2439-01-2 2593-15-9, Etridiazole 2597-03-7, Phenthoate 2631-40-5, Isoprocarb 2921-88-2, Chlorpyrifos 3060-89-7, Metobromuron 3766-81-2, Fenobucarb 4682-03-5, Diazodinitrophenol 4685-14-7, Paraquat 5234-68-4, Carboxin 5598-13-0, Chlorpyrifos methyl 5836-29-3, Coumatetralyl 6923-22-4, Monocrotophos 7287-19-6, Prometryn 7696-12-0, Tetramethrin 9004-70-0, Nitrocellulose 10061-01-5, cis-1,3-Dichloropropylene 10061-02-6, trans-1,3-Dichloropropylene 10605-21-7, Carbendazim 12789-03-6, Chlordane 13071-79-9, Terbufos 13171-21-6, Phosphamidon 13194-48-4, Ethoprophos 13593-03-8, Quinalphos 15299-99-7, Napropamide 15972-60-8, Alachlor 16752-77-5, Methomyl

17109-49-8, Edifenphos 17606-31-4, Bensultap 17804-35-2, Benomyl 18294-04-7 18625-12-2, 2,4-DB methyl ester 19044-88-3, Oryzalin 19666-30-9, Oxadiazon 21087-64-9, Metribuzin 22224-92-6, Fenamiphos 22781-23-3, Bendiocarb 23103-98-2, Pirimicarb 23184-66-9, Butachlor 23564-05-8, Thiophanate-methyl 24579-73-5, Propamocarb 25057-89-0, Bentazone 25311-71-1, Isofenphos
RL: ANT (Analyte); ANST (Analytical study)
(screening of toxic materials by high-performance TLC and GC/MS)

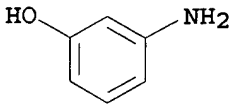
L67 ANSWER 4 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:254083 HCAPLUS
DOCUMENT NUMBER: 132:293329
TITLE: Preparation of amines by solid phase synthesis
INVENTOR(S): Koebberling, Johannes
PATENT ASSIGNEE(S): Germany
SOURCE: Ger. Offen., 8 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19847231	A1	20000420	DE 1998-19847231 <--	19981014
PRIORITY APPLN. INFO.:			DE 1998-19847231 <--	19981014

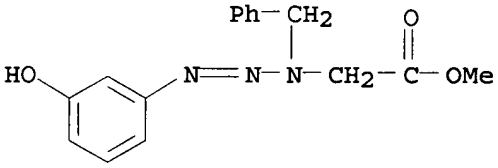
OTHER SOURCE(S): MARPAT 132:293329
AB The title process comprises modification of R1 and/or R2 of R1R2NH (I) by condensation of I with a solid phase-linked diazonium group, carrying out said modification, and cleavage of modified I. Condensation and cleavage of unmodified I was demonstrated.
IT **591-27-5**, 3-Hydroxyaniline
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of amines by solid phase synthesis)
RN 591-27-5 HCAPLUS
CN Phenol, 3-amino- (9CI) (CA INDEX NAME)



IT **591-27-5DP**, 3-Hydroxyaniline, resin bound
264230-86-6DP, resin bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of amines by solid phase synthesis)
RN 591-27-5 HCAPLUS
CN Phenol, 3-amino- (9CI) (CA INDEX NAME)



RN 264230-86-6 HCAPLUS
CN Acetic acid, [3-(3-hydroxyphenyl)-1-(phenylmethyl)-2-triazenyl]-, methyl ester (9CI) (CA INDEX NAME)



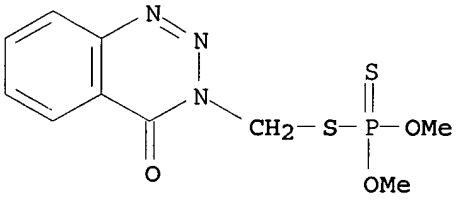
IC ICM C07B043-06
CC 21-2 (General Organic Chemistry)
IT 100-46-9, Benzylamine, reactions 110-85-0, Piperazine, reactions 124-02-7, Diallylamine **591-27-5**, 3-Hydroxyaniline 53386-64-4, Glycine, N-phenylmethyl-, methyl ester
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of amines by solid phase synthesis)
IT 369-61-9DP, resin bound **591-27-5DP**, 3-Hydroxyaniline, resin bound 264230-83-3DP, resin bound 264230-84-4DP, resin bound 264230-85-5DP, resin bound **264230-86-6DP**, resin bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of amines by solid phase synthesis)
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L67 ANSWER 5 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:410761 HCAPLUS
DOCUMENT NUMBER: 131:218822
TITLE: Estimation of Organic Carbon Normalized Sorption Coefficient (KOC) for Soils Using the Fragment Constant Method
AUTHOR(S): Tao, Shu; Piao, Haishan; Dawson, R.; Lu, Xiaoxia; Hu, Haiying
CORPORATE SOURCE: Department of Urban and Environmental Sciences, Peking University, Beijing, 100871, Peop. Rep. China
SOURCE: Environmental Science and Technology (**1999**), 33(16), 2719-2725
CODEN: ESTHAG; ISSN: 0013-936X
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A fragment const. model for prediction of KOC was developed and evaluated with a diverse database of 592 chems. belonging to 17 classes. The range of exptl. KOC covered 7.65 log-units. The 592 chems. were randomly divided into a training set and a testing set for model development and validation. A general model was then established using the entire database having 74 fragment consts. and

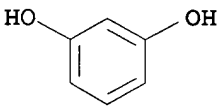
24 structural factors. Statistically, the regression model accounted for as much as 96.96% of the variation in the measured log KOC. The mean residual between the exptl. and predicted KOC values was 0.366 log-units. In >74% of the chems. studied the residual values were <0.5 log-units. The robustness of the regression model, with respect to either specific individual chems. or particular compd. classes, was evaluated through use of jackknife tests. The results confirmed the ability of the fragment model to predict KOC for a wide variety of untested chems.

IT **86-50-0**, Azinphos-methyl **108-46-3**, 1,3-Dihydroxybenzene, occurrence
RL: POL (Pollutant); PRP (Properties); OCCU (Occurrence)
(estn. of org. carbon normalized sorption coeff. for soils using fragment const. method)

RN 86-50-0 HCAPLUS
CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



CC 61-2 (Water)
Section cross-reference(s): 19, 60

IT 50-00-0, Formaldehyde, occurrence 50-29-3, occurrence 50-32-8, Benzo[a]pyrene, occurrence 51-66-1, 4-Methoxyacetanilide 52-68-6, Trichlorfon 53-70-3, Dibenz[a,h]anthracene 55-21-0, Benzamide 55-38-9, Fenthion 56-23-5, occurrence 56-38-2, O,O-Diethyl-O-p-nitrophenyl phosphorothioate 56-49-5, 3-Methylcholanthrene 56-55-3, Benz[a]anthracene 57-13-6, Urea, occurrence 57-55-6, 1,2-Propanediol, occurrence 57-97-6 58-89-9, Lindane 58-90-2, 2,3,4,6-Tetrachlorophenol 60-51-5, O,O-Dimethyl S-(N-methylcarbamoylmethyl)phosphorodithioate 60-57-1, Dieldrin 61-82-5, 1H-1,2,4-Triazol-3-amine 62-23-7, 4-Nitrobenzoic acid 62-53-3, Benzenamine, occurrence 62-73-7, 2,2-Dichlorovinyl dimethyl phosphate 63-25-2, Carbaryl 63-99-0, 3-Methylphenylurea 64-10-8, Phenylurea 64-17-5, Ethanol, occurrence 64-19-7, Acetic acid, occurrence 65-85-0, Benzoic acid, occurrence 67-56-1, Methanol, occurrence 67-66-3, Trichloromethane, occurrence 67-72-1, Hexachloroethane 71-23-8, 1-Propanol, occurrence 71-36-3, 1-Butanol, occurrence 71-41-0, 1-Pentanol, occurrence 71-43-2, Benzene, occurrence 71-55-6, 1,1,1-Trichloroethane 72-54-8 72-55-9, occurrence 75-09-2, occurrence 75-21-8, Oxirane, occurrence 75-25-2, Tribromomethane

75-27-4, Bromodichloromethane 75-34-3, 1,1-Dichloroethane
75-35-4, 1,1-Dichloroethylene, occurrence 75-50-3, Trimethylamine,
occurrence 75-69-4, Trichlorofluoromethane 75-99-0,
2,2-Dichloropropionic acid 76-44-8 77-47-4,
Hexachlorocyclopentadiene 78-75-1, 1,2-Dibromopropane 78-87-5,
1,2-Dichloropropane 79-00-5, 1,1,2-Trichloroethane 79-01-6,
Trichloroethylene, occurrence 79-34-5, 1,1,2,2-Tetrachloroethane
82-68-8, Pentachloronitrobenzene 83-32-9, Acenaphthene 84-66-2,
Diethyl phthalate 84-74-2, Dibutyl phthalate 85-01-8,
Phenanthrene, occurrence 85-02-9, Benzo[f]quinoline 85-34-7,
Fenac 85-68-7, Butyl-benzyl phthalate **86-50-0**,
Azinphos-methyl 86-73-7, Fluorene 86-74-8, 9H-Carbazole
86-87-3, 1-Naphthylacetic acid 87-86-5, Pentachlorophenol
88-06-2, 2,4,6-Trichlorophenol 88-75-5 88-85-7,
2-sec-Butyl-4,6-dinitrophenol 88-99-3, Phthalic acid, occurrence
90-05-1, o-Methoxyphenol 90-12-0, 1-Methylnaphthalene 90-15-3,
1-Naphthol 91-16-7, 1,2-Dimethoxybenzene 91-20-3, Naphthalene,
occurrence 91-22-5, Quinoline, occurrence 91-57-6,
2-Methylnaphthalene 91-66-7, N,N-Diethylaniline 91-94-1,
3,3'-Dichlorobenzidine 92-24-0, Tetracene 92-52-4, Biphenyl,
occurrence 92-82-0, Phenazine 92-87-5, Benzidine 92-91-1,
4-Acetylbiphenyl 93-08-3 93-58-3, Methyl benzoate 93-72-1,
2-(2,4,5-Trichlorophenoxy)propionic acid 93-76-5,
2,4,5-Trichlorophenoxyacetic acid 93-89-0, Ethyl benzoate
93-99-2, Phenyl benzoate 94-08-6, Ethyl 4-methylbenzoate
94-75-7, 2,4-Dichlorophenoxyacetic acid, occurrence 94-82-6,
2,4-DB 95-14-7, 1H-Benzotriazole 95-15-8, Benzo[b]thiophene
95-47-6, 1,2-Dimethylbenzene, occurrence 95-48-7, occurrence
95-49-8, o-Chlorotoluene 95-50-1, 1,2-Dichlorobenzene 95-57-8,
o-Chlorophenol 95-63-6, 1,2,4-Trimethylbenzene 95-76-1,
3,4-Dichloroaniline 95-77-2, 3,4-Dichlorophenol 95-93-2,
1,2,4,5-Tetramethylbenzene 95-94-3, 1,2,4,5-Tetrachlorobenzene
95-95-4, 2,4,5-Trichlorophenol 98-16-8, 3-Trifluoromethylaniline
98-85-1, sec-Phenethyl alcohol 98-86-2, Acetophenone, occurrence
98-95-3, Nitrobenzene, occurrence 99-09-2, 3-Aminonitrobenzene
99-30-9, 2,6-Dichloro-4-nitroaniline 99-34-3, 3,5-Dinitrobenzoic
acid 99-35-4, 1,3,5-Trinitrobenzene 99-54-7,
3,4-Dichloronitrobenzene 99-77-4, Ethyl 4-nitrobenzoate 99-94-5,
4-Methylbenzoic acid 99-96-7, 4-Hydroxybenzoic acid, occurrence
100-01-6, occurrence 100-02-7, p-Nitrophenol, occurrence
100-41-4, Ethylbenzene, occurrence 100-42-5, occurrence
100-51-6, Benzyl alcohol, occurrence 100-61-8, N-Methylaniline,
occurrence 100-66-3, Anisole, occurrence 101-05-3 101-21-3,
Isopropyl N-(3-chlorophenyl)carbamate 101-42-8,
1,1-Dimethyl-3-phenylurea 101-84-8, Diphenyl ether 101-97-3,
Ethylphenylacetate 101-99-5, Ethyl N-phenylcarbamate 102-25-0,
1,3,5-Triethylbenzene 103-33-3, Diphenyl diimide 103-65-1,
Propylbenzene 103-82-2, Phenylacetic acid, occurrence 103-84-4,
Acetanilide 103-88-8, p-Bromoacetanilide 104-51-8, Butylbenzene
106-30-9, Ethyl heptanoate 106-32-1, Ethyl octanoate 106-40-1,
4-Bromoaniline 106-41-2, 4-Bromophenol 106-42-3,
1,4-Dimethylbenzene, occurrence 106-44-5, occurrence 106-46-7,
1,4-Dichlorobenzene 106-47-8, 4-Chloroaniline, occurrence
106-48-9, p-Chlorophenol 106-49-0, 4-Methylaniline, occurrence
106-93-4, 1,2-Dibromoethane 107-02-8, 2-Propenal, occurrence
107-06-2, occurrence 108-38-3, 1,3-Dimethylbenzene, occurrence
108-39-4, occurrence 108-43-0 108-44-1, 3-Methylaniline,
occurrence **108-46-3**, 1,3-Dihydroxybenzene, occurrence
108-67-8, 1,3,5-Trimethylbenzene, occurrence 108-68-9,
3,5-Dimethylphenol 108-70-3, 1,3,5-Trichlorobenzene 108-86-1,

Bromobenzene, occurrence 108-88-3, Toluene, occurrence 108-90-7, Chlorobenzene, occurrence 108-95-2, Phenol, occurrence 109-73-9, 1-Butylamine, occurrence 111-27-3, 1-Hexanol, occurrence 111-44-4, Bis(2-chloroethyl) ether 111-70-6, 1-Heptanol 111-87-5, 1-Octanol, occurrence 112-30-1, 1-Decanol 112-53-8, 1-Dodecanol 114-26-1, Propoxur 114-38-5, 2-Chlorophenylurea 115-29-7, Endosulfan 115-32-2, Dicofol 115-90-2, Fensulfothion 116-06-3, 2-Methyl-2-(methylthio)propionaldehyde O-(methylcarbamoyl)oxime 117-18-0 117-81-7, Bis(2-ethylhexyl) phthalate 118-74-1 118-96-7, 2,4,6-Trinitrotoluene 119-61-9, Benzophenone, occurrence 119-91-5, 2,2'-Biquinoline 120-12-7, Anthracene, occurrence 120-36-5, Dichlorprop 120-47-8, Ethyl 4-hydroxybenzoate 120-80-9, o-Dihydroxybenzene, occurrence 120-82-1, 1,2,4-Trichlorobenzene 120-83-2, 2,4-Dichlorophenol 121-69-7, occurrence 121-75-5, Malathion 121-81-3, 3,5-Dinitrobenzamide 122-14-5, Fenitrothion 122-28-1 122-34-9 122-39-4, Diphenylamine, occurrence 122-42-9, Isopropyl carbanilate 123-33-1, Maleic hydrazide 123-66-0, Ethyl hexanoate 124-40-3, occurrence 124-48-1, Dibromochloromethane 127-18-4, Tetrachloroethylene, occurrence 129-00-0, Pyrene, occurrence 131-11-3, Dimethyl phthalate 132-65-0, Dibenzothiophene 132-66-1, Naptalam 133-07-3, N-(Trichloromethylthio)phthalimide 133-90-4, 3-Amino-2,5-dichlorobenzoic acid 134-32-7, 1-Naphthylamine 136-60-7, Butyl benzoate 139-40-2, 2-Chloro-4,6-bis(isopropylamino)-s-triazine 141-66-2, Dicrotophos 142-62-1, Hexanoic acid, occurrence 143-08-8, 1-Nonanol 148-79-8, Thiabendazole 150-13-0, 4-Aminobenzoic acid 150-19-6 150-68-5 150-76-5, p-Methoxyphenol 156-60-5, trans-1,2-Dichloroethylene 191-24-2, Benzo[ghi]perylene 192-97-2, Benzo[e]pyrene 193-39-5, Indeno(1,2,3-cd)pyrene 194-59-2, 7H-Dibenzo(c,g)carbazole 198-55-0, Perylene 205-99-2, Benz[e]acephenanthrylene 206-44-0, Fluoranthene 207-08-9, Benzo[k]fluoranthene 218-01-9, Chrysene 224-41-9, Dibenz[a,j]anthracene 238-84-6, 1,2-Benzofluorene 239-64-5, 13H-Dibenzo(a,i)carbazole 260-94-6, Acridine 298-00-0, O,O-Dimethyl-O-p-nitrophenyl phosphorothioate 298-02-2, O,O-Diethyl S-[(ethylthio)methyl] phosphorodithioate 298-04-4, Disulfoton

RL: POL (Pollutant); PRP (Properties); OCCU (Occurrence)
(estn. of org. carbon normalized sorption coeff. for soils using fragment const. method)

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L67 ANSWER 6 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:190808 HCAPLUS
DOCUMENT NUMBER: 130:256527
TITLE: Incorporation of potential for multi-media exposure into chemical hazard scores for pollution prevention
AUTHOR(S): Whaley, David A.; Meloy, Thomas P.; Barrett, Shayla S.; Bedillion, Erik J.
CORPORATE SOURCE: Department of Industrial Management Systems Engineering, Safety and Environmental Management Program, West Virginia University, Morgantown, WV, 26506, USA
SOURCE: Drug and Chemical Toxicology (1977) (**1999**), 22(1), 241-273
CODEN: DCTODJ; ISSN: 0148-0545

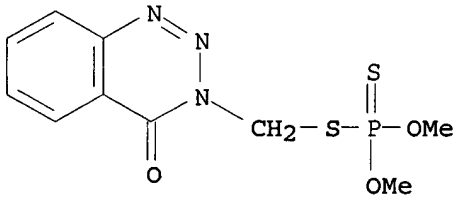
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A chem. hazard score for pollution prevention, the Purdue score, is described. This score provides a relative quant. measure by combining a variety of chem. hazards into a single quant. hazard weighting factor for the non-expert to use. Major expected uses are safer product design, implementing and measuring pollution prevention, and as an adjunct for reporting Toxic Release Inventory data to USEPA. Scoring results are presented for 200 Superfund chems., rank-ordered by worker and environmental hazard, and by combined worker and environmental hazard scores. The extent to which the Purdue score incorporates potential for multi-media pathway and multi-route absorption exposure is discussed. Until other possible uses are tested, peer-reviewed, and published, users are advised to limit this system to planning, implementing, and measuring pollution prevention and enhancing interpretation of Toxic Release Inventory data. How the structure of this score handles exposure to chems., via multi-compartment pathways and multi-routes, for contact or absorption health damage, and how it handles habitat degrdn. by chems. is given. For all of these, the approach is built on inherent properties of each chem. true for all sites and scenarios. The largest obstacle to scoring is lack of measured chem. property data. Missing data is handled by regression, quant. structure activity relationship estns., and a missing data default rule. Limitations of chem. hazard scoring are discussed. Currently, there is no widely accepted single measure of relative chem. hazard, against which to calibrate this hazard score for accuracy, except experience from industrial use. Despite limitations, is is suggested there is a strong value added for industry and society in an available concise, simple-to-use measure of relative chem. hazards. The Purdue score enables sep. or combined consideration of chem. hazard to workers and the environment. It has potential for major cost savings in relative hazard ranking and business decision-making concerning little-studied org. chems. due to the extensive use of advanced property estn. software. This tool is now ready for pilot use by industry. It is mainly intended to assist and encourage businesses to implement and measure pollution prevention cost-effectively. It relies strongly on sub-lethal toxicity; there is practical potential for it to be used with thousands of chems.

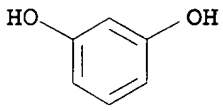
IT **86-50-0**, Guthion **108-46-3**, Resorcinol, biological studies
RL: ADV (Adverse effect, including toxicity); POL (Pollutant); TEM (Technical or engineered material use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(incorporating potential health and environmental hazards from multi-media chem. exposure into chem. hazard Purdue scores for pollution prevention)

RN 86-50-0 HCAPLUS

CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



CC 59-5 (Air Pollution and Industrial Hygiene)
Section cross-reference(s): 4, 20, 45, 49
IT 50-29-3, DDT, biological studies 50-32-8, Benzo(a)pyrene, biological studies 51-79-6, Urethane 55-63-0, Nitroglycerin 55-86-7, Nitrogen mustard 55-91-4 56-38-2, Parathion 56-53-1, Diethylstilbestrol 56-55-3, Benzo(a)anthracene 57-14-7, 1,1-Dimethylhydrazine 57-24-9, Strychnine 57-57-8, β-Propiolactone 57-97-6, 7,12-Dimethylbenz(a)anthracene 58-89-9, Lindane 60-11-7, 4-Dimethylaminoazobenzene 60-29-7, Ethyl ether, biological studies 60-34-4, Methylhydrazine 60-35-5, Acetamide, biological studies 60-51-5, Dimethoate 60-57-1, Dieldrin 61-82-5, Amitrole 62-38-4, Phenylmercuric acetate 62-44-2, Phenacetin 62-56-6, Thiocarbamide, biological studies 62-73-7, Dichlorvos 62-75-9 64-18-6, Formic acid, biological studies 64-19-7, Acetic acid, biological studies 68-12-2, Dimethylformamide, biological studies 70-30-4, Hexachlorophene 72-20-8, Endrin 72-43-5, Methoxychlor 74-88-4, Iodomethane, biological studies 74-89-5, Methylamine, biological studies 74-93-1, Methanethiol, biological studies 75-04-7, Ethylamine, biological studies 75-25-2, Bromoform 75-34-3, Ethylidene chloride 75-44-5, Phosgene 75-50-3, Trimethylamine, biological studies 75-55-8 75-64-9, tert-Butylamine, biological studies 75-71-8, Dichlorodifluoromethane 75-86-5, Acetone cyanohydrin 76-44-8, Heptachlor 77-47-4, Hexachlorocyclopentadiene 77-78-1, Dimethyl sulfate 78-00-2, Tetraethyl lead 78-59-1, Isophorone 78-79-5, Isoprene, biological studies 78-81-9, Isobutylamine 78-83-1, Isobutyl alcohol, biological studies 79-09-4, Propionic acid, biological studies 79-11-8, Chloroacetic acid, biological studies 79-19-6, Hydrazine carbothioamide 79-34-5, 1,1,2,2-Tetrachloroethane 79-44-7, Dimethyl carbamoyl chloride 81-81-2, Warfarin 82-68-8, Quintozene **86-50-0**, Guthion 87-86-5, Pentachlorophenol 88-06-2, 2,4,6-Trichlorophenol 88-85-7, Dinoseb 91-22-5, Quinoline, biological studies 92-67-1, 4-Aminobiphenyl 92-87-5, Benzidine 93-76-5, 2,4,5-Trichlorophenoxyacetic acid 95-48-7, o-Cresol, biological studies 95-53-4, o-Toluidine, biological studies 95-95-4, 2,4,5-Trichlorophenol 96-09-3, Styrene oxide 96-12-8, DBCP 96-45-7, Ethylene thiourea 98-01-1, Furfural, biological studies 98-86-2, Acetophenone, biological studies 98-87-3, Benzal chloride 99-35-4, 1,3,5-Trinitrobenzene

100-01-6, biological studies 100-44-7, Benzyl chloride, biological studies 100-75-4 101-14-4, MOCA 103-85-5, Phenylthiourea 105-60-2, Caprolactam, biological studies 106-47-8, biological studies 106-51-4, Quinone, biological studies 106-88-7, 1,2-Butylene oxide 106-93-4, Ethylene dibromide 107-02-8, Acrolein, biological studies 107-15-3, Ethylenediamine, biological studies 107-18-6, Allyl alcohol, biological studies 107-19-7, Propargyl alcohol 107-20-0, Chloroacetaldehyde 107-30-2, Chloromethyl methyl ether 107-49-3, Tepp 108-24-7, Acetic anhydride **108-46-3**, Resorcinol, biological studies 108-94-1, Cyclohexanone, biological studies 108-98-5, Benzenethiol, biological studies 109-06-8, 2-Methylpyridine 109-73-9, Butylamine, biological studies 109-77-3, Malononitrile 109-89-7, Diethylamine, biological studies 109-99-9, Tetrahydrofuran, biological studies 110-00-9, Furan 110-54-3, n-Hexane, biological studies 111-91-1, Bis(2-chloroethoxy)methane 114-26-1, Propoxur 115-29-7, Endosulfan 116-06-3, Aldicarb 121-44-8, Triethylamine, biological studies 122-09-8 123-33-1, Maleic hydrazide 123-86-4, Butyl acetate 123-92-2, Isoamyl acetate 124-40-3, Dimethylamine, biological studies 126-98-7, Methacrylonitrile 131-89-5, 2-Cyclohexyl-4,6-dinitrophenol 137-26-8, Thiram 141-78-6, Ethyl acetate, biological studies 151-50-8, Potassium cyanide 151-56-4, Aziridine, biological studies 152-16-9 225-51-4, Benz(c)acridine 298-02-2, Phorate 298-04-4, Disulfoton 302-01-2, Hydrazine, biological studies 309-00-2, Aldrin 311-45-5, Diethyl-p-nitrophenyl phosphate 315-18-4, Mexacarbate 370-14-9, Isodrin 504-24-5, 4-Aminopyridine 506-64-9, Silver cyanide (Ag(CN)) 506-68-3, Bromine cyanide 506-77-4, Chlorine cyanide 509-14-8, Tetranitromethane 510-15-6, Chlorobenzilate 528-29-0, o-Dinitrobenzene 534-52-1, 4,6-Dinitro-o-cresol 540-73-8, 1,2-Dimethylhydrazine 542-88-1, Bis(chloromethyl)ether 563-12-2, Ethion 593-60-2, Vinyl bromide 594-42-3, Perchloromethyl mercaptan 598-03-8 606-20-2, 2,6-Dinitrotoluene 608-93-5, Pentachlorobenzene 610-39-9, 3,4-Dinitrotoluene 624-83-9, Methyl isocyanate 628-63-7, n-Amyl acetate 680-31-9, Hexamethylphosphoramide, biological studies 684-93-5 764-41-0, 1,4-Dichloro-2-butene 765-34-4, Glycidaldehyde 822-06-0, Hexamethylene-1,6-Diisocyanate 1314-62-1, Vanadium pentoxide, biological studies 1327-53-3, Arsenic trioxide 1338-23-4, Methyl ethyl ketone peroxide 1404-00-8, Mitomycin 1464-53-5, Diepoxybutane 1563-66-2, Carbofuran 2074-87-5, Cyanogen 2303-16-4, Diallate 2465-27-2, Auramine 3689-24-5 4170-30-3, 2-Butenal 4549-40-0 5344-82-1, 2-Chlorophenylthiourea 7439-92-1, Lead, biological studies 7440-41-7, Beryllium, biological studies 7440-50-8, Copper, biological studies 7446-18-6, Thallous sulfate 7647-18-9, Antimony pentachloride 7719-12-2, Phosphorus trichloride 7778-39-4, Arsenic acid 7782-41-4, Fluorine, biological studies 7783-06-4, Hydrosulfuric acid, biological studies 7783-56-4, Antimony trifluoride 7786-34-7, Mevinphos 7789-61-9, Antimony tribromide 7803-51-2, Phosphine 8001-35-2, Camphechlor 10025-87-3, Phosphorus oxychloride 10099-74-8, Lead nitrate 10102-43-9, Nitric oxide, biological studies 10102-44-0, Nitrogen dioxide, biological studies 12789-03-6, Chlordane 13463-39-3, Nickel carbonyl 13952-84-6, sec-Butylamine 16752-77-5, Methomyl 25321-14-6, Dinitrotoluene 26628-22-8, Sodium azide 26952-23-8, Dichloropropene 30525-89-4, Paraformaldehyde 41903-57-5, Tetrachlorodibenzo-p-dioxin 61970-39-6, Osmium oxide
RL: ADV (Adverse effect, including toxicity); POL (Pollutant); TEM

(Technical or engineered material use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(incorporating potential health and environmental hazards from multi-media chem. exposure into chem. hazard Purdue scores for pollution prevention)

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

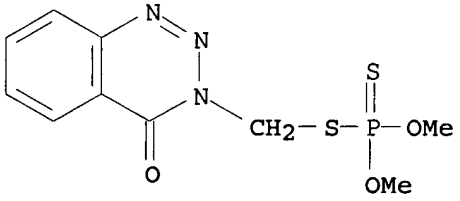
L67 ANSWER 7 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:778677 HCAPLUS
DOCUMENT NUMBER: 128:44769
TITLE: Allergic contact sensitizing chemicals as environmental carcinogens
AUTHOR(S): Albert, Roy E.
CORPORATE SOURCE: Department of Environmental Health, University of Cincinnati Medical Center, Cincinnati, OH, 45267-0056, USA
SOURCE: Environmental Health Perspectives (**1997**), 105(9), 940-948
CODEN: EVHPAZ; ISSN: 0091-6765
PUBLISHER: National Institute of Environmental Health Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Chems. that were bioassayed by the National Toxicol. Program (NTP) and that also produce allergic dermatitis (ACD) in humans were evaluated for their tumorigenic characteristics. The impetus for the study was that most contact sensitizers, i.e., those that produce ACD, and genotoxic carcinogens are chem. similar in that they are electrophilic, thereby producing adducts on macro-mols. including protein and DNA. This similarity in chem. behavior suggests that many contact sensitizers might be environmental carcinogens. All of the published NTP bioassays by early 1996 that had both genotoxicity and carcinogenicity studies were included in this anal. The NTP chems. had been chosen for bioassay without regard to their ability to produce ACD. Of the 209 chems. that were bioassayed, there were 36 (17%) that were known to be human contact sensitizers; about half of these were pos. on tumor bioassays. The contact sensitizers differed from the NTP sample as a whole by having a proportionately larger no. of nongenotoxic chems. by the Ames Salmonella assay, presumably because more of them were selected on the basis of widespread usage rather than structural resemblance to known carcinogens. Compared to the nongenotoxic chems., the genotoxics were stronger carcinogens in that they had a higher incidence of pos. tumor bioassays, with twice the no. of organs in which tumors were induced. The nongenotoxic chems. had a preference for tumor induction in parenchymal tissues in contrast to epithelial tissues. The contact sensitizers showed essentially the same characteristics as the whole NTP sample when stratified according to genotoxicity. Judging by the chems. that were chosen primarily for their widespread use rather than for their structural resemblance to carcinogens, the addn. of a test for contact sensitization to the Ames test as a screening tool would increase the tumorigenic detection efficiency by about 40% because of the nongenotoxic tumorigens. A ballpark est. suggests that there could be several thousand contact sensitizers for humans in com. use that are rodent tumorigens.

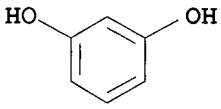
IT **86-50-0 108-46-3**, 1,3-Benzenediol, biological studies **140-56-7**

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(allergic contact sensitizing chems. as environmental carcinogens)

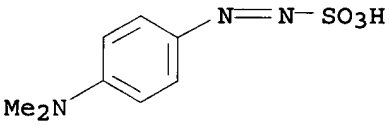
RN 86-50-0 HCAPLUS
CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



RN 140-56-7 HCAPLUS
CN Diazenesulfonic acid, [4-(dimethylamino)phenyl]-, sodium salt (9CI) (CA INDEX NAME)



● Na

CC 4-3 (Toxicology)
IT 50-33-9, biological studies 54-31-9 55-38-9 56-38-2 57-06-7 57-41-0 58-14-0 62-73-7 63-92-3 67-66-3, biological studies 71-55-6 72-56-0 74-96-4 75-09-2, biological studies 75-25-2 75-47-8 75-56-9, biological studies 76-01-7 76-06-2 76-44-8 77-47-4 77-65-6 78-34-2 78-42-2, Tris(2-ethylhexyl)phosphate 78-59-1 78-87-5 79-00-5 79-01-6, biological studies 80-08-0 80-62-6 82-28-0 82-68-8 **86-50-0** 87-29-6 87-62-7, 2,6-Xylidine 87-86-5 91-20-3, Naphthalene, biological studies 91-64-5, 2H-1-Benzopyran-2-one 91-93-0 95-14-7, 1H-Benzotriazole 95-50-1 95-80-7, 2,4-Diaminotoluene 95-83-0 96-12-8 96-13-9 96-18-4 96-45-7, 2-Imidazolidinethione 96-48-0 97-53-0 97-77-8 98-01-1, 2-Furancarboxaldehyde, biological studies 98-85-1 99-55-8 99-56-9 99-57-0 99-59-2 100-02-7, biological studies 100-51-6, Benzenemethanol, biological studies 101-54-2 101-80-4 101-90-6 102-50-1 102-96-5 103-23-1

103-33-3 103-85-5 103-90-2 105-11-3 106-46-7 106-47-8,
biological studies 106-87-6 106-88-7 106-92-3 106-93-4
107-06-2, biological studies 107-07-3, biological studies
108-46-3, 1,3-Benzenediol, biological studies 108-60-1
108-95-2, Phenol, biological studies 110-00-9, Furan 113-92-8
117-39-5 117-79-3 117-81-7 118-92-3 119-34-6 119-53-9
120-71-8 121-14-2 121-66-4 121-69-7, biological studies
121-75-5 121-79-9 121-88-0 122-66-7 123-31-9,
1,4-Benzenediol, biological studies 124-64-1 127-18-4,
biological studies 127-69-5 131-17-9 132-32-1 133-06-2
135-20-6 136-40-3 137-09-7 137-17-7 137-30-4 139-65-1
139-94-6 140-11-4 140-49-8 **140-56-7** 140-88-5
147-24-0 148-24-3, 8-Quinolinol, biological studies 149-30-4,
2(3H)-Benzothiazolethione 150-68-5 156-10-5 156-62-7
298-00-0 298-59-9, Methylphenidate hydrochloride 303-34-4
320-67-2 458-37-7, Curcumin 504-88-1 509-14-8,
Tetranitromethane 512-56-1 513-37-1 532-27-4 542-75-6
556-52-5, Oxiranemethanol 563-47-3 569-61-9 597-25-1
609-20-1 615-05-4 624-18-0 828-00-2 842-07-9 868-85-9
924-42-5 989-38-8 1067-33-0 1582-09-8 1634-78-2, Maloxon
1746-01-6 1777-84-0 1825-21-4 1836-75-5, Nitrofen 1897-45-6,
Chlorothalonil 1918-02-1 1936-15-8 2185-92-4 2244-16-8
2425-85-6 2432-99-7 2475-45-8 2783-94-0 2784-94-3
2832-40-8 2835-39-4 2871-01-4 3165-93-3 5131-60-2
5160-02-1 5307-14-2 5634-39-9 6369-59-1 6373-74-6
6459-94-5 6471-49-4 6959-47-3 6959-48-4 7446-34-6, Selenium
sulfide (SeS) 7487-88-9, Magnesium sulfate, biological studies
7487-94-7, Mercury chloride (HgCl2), biological studies 7681-49-4,
Sodium fluoride (NaF), biological studies 7772-99-8, Tin chloride
(SnCl2), biological studies 9005-65-6 11084-85-8, Sodium
hypochlorite phosphate (Na13(ClO)(PO4)4) 13366-73-9 13463-67-7,
Titanium oxide (TiO2), biological studies 15481-70-6 17026-81-2
17924-92-4 19010-66-3 21739-91-3 26471-62-5 33229-34-4
54150-69-5 55566-30-8 59820-43-8 61702-44-1
RL: ADV (Adverse effect, including toxicity); BIOL (Biological
study)
(allergic contact sensitizing chems. as environmental
carcinogens)

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L67 ANSWER 8 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:681558 HCAPLUS
DOCUMENT NUMBER: 127:273987
TITLE: Feed forward back-propagation neural networks and their use in predicting the acute toxicity of chemicals to the fathead minnow. [Erratum to document cited in CA127:132092]
AUTHOR(S): Kaiser, Klaus L. E.; Niculescu, Stefan P.; Schuurmann, Gerrit
CORPORATE SOURCE: National Water Research Institute, Environment Canada, Burlington, ON, L7R 4A6, Can.
SOURCE: Water Quality Research Journal of Canada (**1997**), 32(4), 855
CODEN: WQRCFA; ISSN: 1201-3080
PUBLISHER: Canadian Association on Water Quality
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Printing errors are noted for lines 32-33 on page 642; line 29 on

page 643; lines 5,6, and 9 on page 644; line 17 on page 648; line 3 on page 649; lines 1 and 3 on page 649; and line 1 on page 650. The errors involved capitalization, subscript/superscript use, and use of # rather than ≤ with variables and equations.

IT **86-50-0**, Azinphos-methyl **108-46-3**, Resorcinol, biological studies
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(feed forward backpropagation neural networks and use in predicting acute toxicity of chems. to fathead minnow (Erratum))

RN 86-50-0 HCAPLUS
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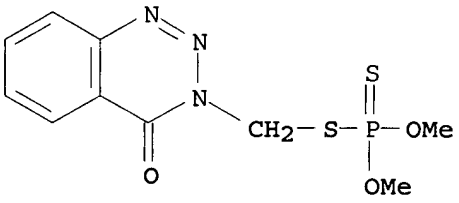
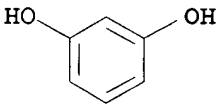


RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



CC 4-3 (Toxicology)

IT 50-00-0, Formaldehyde, biological studies 50-29-3, p,p'-Ddt, biological studies 51-28-5, 2,4-Dinitrophenol, biological studies 51-79-6, Urethane 52-68-6, Trichlorfon 55-18-5, N-Nitrosodiethylamine 55-21-0, Benzamide 56-23-5, Carbon tetrachloride, biological studies 56-35-9, Bis(tributyltin)oxide 56-37-1, Benzyltriethylammonium chloride 56-38-2, Parathion-ethyl 57-06-7, Allyl isothiocyanate 57-15-8, Chloretone 57-43-2, Amytal 58-08-2, Caffeine, biological studies 58-27-5, 2-Methyl-1,4-naphthoquinone 58-89-9, Lindane 58-90-2, 2,3,4,6-Tetrachlorophenol 59-50-7, 4-Chloro-3-methylphenol 60-29-7, Diethyl ether, biological studies 60-57-1, Dieldrin 62-53-3, Aniline, biological studies 62-73-7, Dichlorvos 63-25-2, Carbaryl 64-17-5, Ethanol, biological studies 64-19-7, Acetic acid, biological studies 66-25-1, Hexanal 67-56-1, Methanol, biological studies 67-63-0, 2-Propanol, biological studies 67-64-1, Acetone, biological studies 67-66-3, Chloroform, biological studies 67-68-5, Dimethyl sulfoxide, biological studies 67-72-1, Hexachloroethane 68-12-2, N,N-Dimethylformamide, biological studies 70-30-4, Hexachlorophene 71-23-8, 1-Propanol, biological studies 71-36-3, 1-Butanol, biological studies 71-41-0, 1-Pentanol, biological studies 71-43-2, Benzene, biological studies 71-55-6, 1,1,1,-Trichloroethane 74-90-8, Hydrogen cyanide, biological studies 75-05-8, Acetonitrile, biological studies 75-07-0, Acetaldehyde, biological studies 75-09-2, Dichloromethane, biological studies

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4-Toluidine, biological studies 106-51-4, 1,4-Benzoquinone, biological studies 106-89-8, Epichlorohydrin, biological studies 107-02-8, Acrolein, biological studies 107-06-2, 1,2-Dichloroethane, biological studies 107-07-3, 2-Chloroethanol, biological studies 107-10-8, Propylamine, biological studies 107-12-0, Propionitrile 107-13-1, Acrylonitrile, biological studies 107-14-2, Chloroacetonitrile 107-15-3, Ethylenediamine, biological studies 107-18-6, Allyl alcohol, biological studies 107-21-1, 1,2-Ethanediol, biological studies 107-22-2, Glyoxal 107-41-5, 2-Methyl-2,4-pentanediol 107-45-9, 1,1,3,3-Tetramethylbutylamine 108-10-1, 4-Methyl-2-pentanone 108-20-3, Diisopropyl ether 108-38-3, biological studies 108-39-4, biological studies 108-41-8, 3-Chlorotoluene **108-46-3**, Resorcinol, biological studies 108-59-8, Dimethyl malonate 108-70-3, 1,3,5-Trichlorobenzene 108-86-1, Bromobenzene, biological studies 108-88-3, Toluene, biological studies 108-89-4, 4-Picoline 108-90-7, Chlorobenzene, biological studies 108-93-0, Cyclohexanol, biological studies 108-94-1, Cyclohexanone, biological studies 108-95-2, Phenol, biological studies 108-99-6, 3-Picoline 109-06-8, 2-Picoline 109-21-7, Butyl butyrate 109-60-4, Propyl acetate 109-73-9, Butylamine, biological studies 109-75-1, Allyl cyanide 109-77-3, Malononitrile 109-85-3, 2-Methoxyethylamine 109-87-5, Dimethoxymethane 109-89-7, Diethylamine, biological studies 109-97-7, Pyrrole 109-99-9, Tetrahydrofuran, biological studies 110-00-9, Furan 110-12-3, 5-Methyl-2-hexanone 110-40-7, Diethyl sebacate 110-54-3, Hexane, biological studies 110-86-1, Pyridine, biological studies 110-93-0, 6-Methyl-5-hepten-2-one 111-13-7, 2-Octanone 111-15-9, 2-Ethoxyethyl acetate 111-26-2, Hexylamine 111-27-3, 1-Hexanol, biological studies 111-42-2, Diethanolamine, biological studies 111-46-6, biological studies 111-68-2, Heptylamine 111-69-3, 1,4-Dicyanobutane 111-70-6, 1-Heptanol 111-83-1, 1-Bromooctane 111-86-4, Octylamine 111-87-5, 1-Octanol, biological studies 111-90-0, 2-(2-Ethoxyethoxy)ethanol 112-27-6, Triethylene glycol 112-30-1, 1-Decanol 112-53-8, 1-Dodecanol 112-80-1, 9-Octadecenoic acid (Z)-, biological studies 115-20-8, 2,2,2-Trichloroethanol 115-29-7, Endosulfan 115-32-2, Dicofol 116-06-3, Aldicarb 118-55-8, Phenyl salicylate 118-79-6, 2,4,6-Tribromophenol 118-96-7, 2,4,6-Trinitrotoluene 119-32-4, 4-Methyl-3-nitroaniline 119-34-6, 4-Amino-2-nitrophenol 119-61-9, Benzophenone, biological studies 120-07-0, N-Phenyldiethanolamine 120-80-9, Catechol, biological studies 120-82-1, 1,2,4-Trichlorobenzene
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(feed forward backpropagation neural networks and use in predicting acute toxicity of chems. to fathead minnow (Erratum))

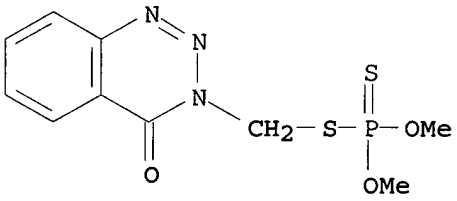
L67 ANSWER 9 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:445203 HCAPLUS
DOCUMENT NUMBER: 127:132092
TITLE: Feed forward backpropagation neural networks and their use in predicting the acute toxicity of chemicals to the fathead minnow
AUTHOR(S): Kaiser, Klaus L.E.; Niculescu, Stefan P.; Schuurmann, Gerrit
CORPORATE SOURCE: National Water Research Institute, Environment Canada, Burlington, ON, L7R 4A6, Can.
SOURCE: Water Quality Research Journal of Canada (**1997**), 32(3), 637-657

CODEN: WQRCFA; ISSN: 1201-3080
PUBLISHER: Canadian Association on Water Quality
DOCUMENT TYPE: Journal
LANGUAGE: English

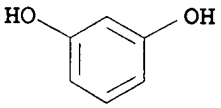
AB Various aspects connected to the use of feed forward backpropagation neural networks to build multivariate QSARs based on large data sets contg. considerable amts. of important information are investigated. Based on such a model and a 419 compd. data set, the explicit equation of one of the resulting multivariate QSARs for the computation of toxicity to the fathead minnow is presented as function of measured Microtox, logarithms of mol. wt. and octanol/water partition coeff., and 48 other functional group and discrete descriptors.

IT **86-50-0**, Azinphos-methyl **108-46-3**, Resorcinol, biological studies
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(feed forward backpropagation neural networks and use in predicting acute toxicity of chems. to fathead minnow)

RN 86-50-0 HCAPLUS
CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



CC 4-3 (Toxicology)

IT 50-00-0, Formaldehyde, biological studies 50-29-3, p,p'-DDT, biological studies 51-28-5, 2,4-Dinitrophenol, biological studies 51-79-6, Urethane 52-68-6, Trichlorfon 55-18-5, N-Nitrosodiethylamine 55-21-0, Benzamide 56-23-5, Carbon tetrachloride, biological studies 56-35-9, Bis(tributyltin)oxide 56-37-1, Benzyltriethylammonium chloride 56-38-2, Parathion-ethyl 57-06-7, Allyl isothiocyanate 57-15-8, Chloretone 57-43-2, Amytal 58-08-2, Caffeine, biological studies 58-27-5, 2-Methyl-1,4-naphthoquinone 58-89-9, Lindane 58-90-2, 2,3,4,6-Tetrachlorophenol 59-50-7, 4-Chloro-3-methylphenol 60-29-7, Diethyl ether, biological studies 60-57-1, Dieldrin 62-53-3, Aniline, biological studies 62-73-7, Dichlorvos 63-25-2, Carbaryl 64-17-5, Ethanol, biological studies 64-19-7, Acetic acid, biological studies 66-25-1, Hexanal 67-56-1, Methanol, biological studies 67-63-0, 2-Propanol, biological studies 67-64-1, Acetone, biological studies 67-66-3,

Chloroform, biological studies 67-68-5, Dimethyl sulfoxide, biological studies 67-72-1, Hexachloroethane 68-12-2, N,N-Dimethylformamide, biological studies 70-30-4, Hexachlorophene 71-23-8, 1-Propanol, biological studies 71-36-3, 1-Butanol, biological studies 71-41-0, 1-Pentanol, biological studies 71-43-2, Benzene, biological studies 71-55-6, 1,1,1,-Trichloroethane 74-90-8, Hydrogen cyanide, biological studies 75-05-8, Acetonitrile, biological studies 75-07-0, Acetaldehyde, biological studies 75-09-2, Dichloromethane, biological studies 75-65-0, 2-Methyl-2-propanol, biological studies 75-89-8, 2,2,2-Trifluoroethanol 75-97-8, 3,3-Dimethylbutan-2-one 76-01-7, Pentachloroethane 76-03-9, Trichloroacetic acid, biological studies 78-27-3, 1-Ethynyl-1-cyclohexanol 78-59-1, Isophorone 78-83-1, 2-Methyl-1-propanol, biological studies 78-87-5, 1,2-Dichloropropane 78-90-0, 1,2-Diaminopropane 78-92-2, 2-Butanol 78-93-3, 2-Butanone, biological studies 78-96-6, 1-Aminopropan-2-ol 79-00-5, 1,1,2-Trichloroethane 79-01-6, Trichloroethylene, biological studies 79-06-1, Acrylamide, biological studies 79-20-9, Methyl acetate 79-34-5, 1,1,2,2-Tetrachloroethane 79-95-8, 4,4'-Isopropylidenebis(2,6-dichlorophenol) 80-62-6, Methyl methacrylate 83-32-9, Acenaphthene 83-79-4, Rotenone 84-62-8, Diphenyl phthalate 84-66-2, Diethyl phthalate 84-74-2, Dibutyl phthalate **86-50-0**, Azinphos-methyl 86-57-7, 1-Nitronaphthalene 87-17-2, Salicylanilide 87-61-6, 1,2,3-Trichlorobenzene 87-86-5 87-91-2, Diethyl L-tartrate, biological studies 88-06-2, 2,4,6-Trichlorophenol 88-30-2, 3-Trifluoromethyl-4-nitrophenol 88-72-2, 2-Nitrotoluene 88-73-3, 1-Chloro-2-nitrobenzene 88-75-5, 2-Nitrophenol 88-85-7, Dinoseb 89-62-3, 4-Methyl-2-nitroaniline 90-02-8, Salicylaldehyde, biological studies 90-12-0, 1-Methylnaphthalene 90-15-3, 1-Naphthol 90-43-7, 2-Phenylphenol 90-47-1, Xanthone 91-20-3, Naphthalene, biological studies 91-22-5, Quinoline, biological studies 91-66-7, N,N-Diethylaniline 92-52-4, Biphenyl, biological studies 93-89-0, Ethyl benzoate 93-91-4, Benzoylacetone 94-09-7, Ethyl-4-aminobenzoate 94-75-7, 2,4-D, biological studies 95-16-9, Benzothiazole 95-47-6, o-Xylene, biological studies 95-48-7, biological studies 95-49-8, 2-Chlorotoluene 95-50-1, 1,2-Dichlorobenzene 95-51-2, 2-Chloroaniline 95-57-8, 2-Chlorophenol 95-65-8, 3,4-Dimethylphenol 95-73-8, 2,4-Dichlorotoluene 95-75-0, 3,4-Dichlorotoluene 95-76-1, 3,4-Dichloroaniline 95-80-7, 2,4-Diaminotoluene 95-94-3, 1,2,4,5-Tetrachlorobenzene 95-95-4, 2,4,5-Trichlorophenol 96-05-9, Allyl methacrylate 96-13-9 96-18-4, 1,2,3-Trichloropropane 96-22-0, 3-Pentanone 96-29-7, 2-Butanone oxime 96-80-0, 2-(Diisopropylamino)ethanol 97-02-9, 2,4-Dinitroaniline 98-54-4, 4-tert-Butylphenol 98-82-8, Isopropylbenzene 98-86-2, Acetophenone, biological studies 98-88-4, Benzoyl chloride 98-95-3, Nitrobenzene, biological studies 99-08-1, 3-Nitrotoluene 99-52-5 99-55-8, 2-Methyl-5-nitroaniline 99-65-0, 1,3-Dinitrobenzene 99-99-0, 4-Nitrotoluene 100-01-6, 4-Nitroaniline, biological studies 100-02-7, 4-Nitrophenol, biological studies 100-10-7, 4-(Dimethylamino)benzaldehyde 100-25-4, 1,4-Dinitrobenzene 100-41-4, Ethylbenzene, biological studies 100-42-5, Styrene, biological studies 100-44-7, Benzyl chloride, biological studies 100-46-9, Benzylamine, biological studies 100-47-0, Benzonitrile, biological studies 100-51-6, Benzyl alcohol, biological studies 100-52-7, Benzaldehyde, biological studies 100-61-8, N-Methylaniline, biological studies 100-64-1, Cyclohexanone oxime

100-70-9, 2-Cyanopyridine 101-84-8, Diphenyl ether 102-08-9, N,N'-Diphenylthiourea 102-27-2 102-71-6, Triethanolamine, biological studies 103-05-9, α,α-Dimethylbenzenepropanol 103-83-3, N,N-Dimethylbenzylamine 103-90-2, 4-Acetamidophenol 104-76-7, 2-Ethyl-1-hexanol 104-88-1, 4-Chlorobenzaldehyde, biological studies 104-90-5, 5-Ethyl-2-methylpyridine 105-67-9, 2,4-Dimethylphenol 105-99-7, Dibutyl adipate 106-42-3, biological studies 106-43-4, 4-Chlorotoluene 106-44-5, biological studies 106-46-7, 1,4-Dichlorobenzene 106-47-8, 4-Chloroaniline, biological studies 106-48-9, 4-Chlorophenol 106-49-0, 4-Toluidine, biological studies 106-51-4, 1,4-Benzoquinone, biological studies 106-89-8, Epichlorohydrin, biological studies 107-02-8, Acrolein, biological studies 107-06-2, 1,2-Dichloroethane, biological studies 107-07-3, 2-Chloroethanol, biological studies 107-10-8, Propylamine, biological studies 107-12-0, Propionitrile 107-13-1, Acrylonitrile, biological studies 107-14-2, Chloroacetonitrile 107-15-3, Ethylenediamine, biological studies 107-18-6, Allyl alcohol, biological studies 107-21-1, Ethylene glycol, biological studies 107-22-2, Glyoxal 107-41-5, 2-Methyl-2,4-pentanediol 107-45-9, 1,1,3,3-Tetramethylbutylamine 108-10-1, 4-Methyl-2-pentanone 108-20-3, Diisopropyl ether 108-38-3, biological studies 108-39-4, biological studies 108-41-8, 3-Chlorotoluene **108-46-3**, Resorcinol, biological studies 108-59-8, Dimethyl malonate 108-70-3, 1,3,5-Trichlorobenzene 108-86-1, Bromobenzene, biological studies 108-88-3, Toluene, biological studies 108-89-4, 4-Picoline 108-90-7, Chlorobenzene, biological studies 108-93-0, Cyclohexanol, biological studies 108-94-1, Cyclohexanone, biological studies 108-95-2, Phenol, biological studies 108-99-6, 3-Picoline 109-06-8, 2-Picoline 109-21-7, Butyl butyrate 109-60-4, Propyl acetate 109-73-9, Butylamine, biological studies 109-75-1, Allyl cyanide 109-77-3, Malononitrile 109-85-3, 2-Methoxyethylamine 109-87-5, Dimethoxymethane 109-89-7, Diethylamine, biological studies 109-97-7, Pyrrole 109-99-9, Tetrahydrofuran, biological studies 110-00-9, Furan 110-12-3, 5-Methyl-2-hexanone 110-40-7, Diethyl sebacate 110-54-3, Hexane, biological studies 110-86-1, Pyridine, biological studies 110-93-0, 6-Methyl-5-hepten-2-one 111-13-7, 2-Octanone 111-15-9, 2-Ethoxyethyl acetate 111-26-2, Hexylamine 111-27-3, 1-Hexanol, biological studies 111-42-2, Diethanolamine, biological studies 111-46-6, Bis(2-hydroxyethyl)ether, biological studies 111-68-2, Heptylamine 111-69-3, 1,4-Dicyanobutane 111-70-6, 1-Heptanol 111-83-1, 1-Bromooctane 111-86-4, Octylamine 111-87-5, 1-Octanol, biological studies 111-90-0, 2-(2-Ethoxyethoxy)ethanol 112-27-6, Triethylene glycol 112-30-1, 1-Decanol 112-53-8, 1-Dodecanol 112-80-1, Oleic acid, biological studies 115-20-8, 2,2,2-Trichloroethanol 115-29-7, Endosulfan 115-32-2, Dicofol 116-06-3, Aldicarb 118-55-8, Phenyl salicylate 118-79-6, 2,4,6-Tribromophenol 118-96-7, 2,4,6-Trinitrotoluene 119-32-4, 4-Methyl-3-nitroaniline 119-34-6, 4-Amino-2-nitrophenol 119-61-9, Benzophenone, biological studies 120-07-0, N-Phenyldiethanolamine 120-80-9, Catechol, biological studies 120-82-1, 1,2,4-Trichlorobenzene
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(feed forward backpropagation neural networks and use in predicting acute toxicity of chems. to fathead minnow)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE

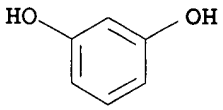
FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L67 ANSWER 10 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:367536 HCAPLUS
DOCUMENT NUMBER: 127:60207
TITLE: Carcinogenicity testing and the evaluation of regulatory requirements for pharmaceuticals
AUTHOR(S): Contrera, Joseph F.; Jacobs, Abigail C.; DeGeorge, Joseph J.
CORPORATE SOURCE: Office Testing and Research and Office of Review Management, U.S. Food and Drug Admin., Center for Drug Evaluation and Research, Rockville, MD, 20857, USA
SOURCE: Regulatory Toxicology and Pharmacology (**1997**), 25(2), 130-145
CODEN: RTOPDW; ISSN: 0273-2300
PUBLISHER: Academic
DOCUMENT TYPE: Journal
LANGUAGE: English

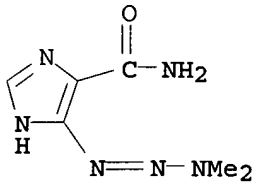
AB Database The results of rat and mouse carcinogenicity studies for 282 human pharmaceuticals in the FDA database were analyzed and compared as part of an International Conference on Harmonization (ICH) evaluation of rodent carcinogenicity studies and their utility for carcinogenicity testing. A majority of the carcinogenicity studies in the FDA database were carried out in Sprague-Dawley-derived rats and Swiss-Webster-derived CD-1 mice in contrast to Fisher 344 rats and B6C3F1 mice employed in National Toxicol. Program (NTP) studies. Despite the differences in rodent strains, the relative proportion of compds. with pos. findings (44.3%) and the degree of overall concordance between rats and mice (74.1%) in the FDA database were similar to the NTP rodent carcinogenicity database. Carcinogenicity studies in two rodent species are necessary primarily to identify trans-species tumorigens, which are considered to pose a relatively greater potential risk to humans than single species pos. compds. Two-year carcinogenicity studies in both rats and mice may not be the only means of identifying transspecies tumorigens. Sufficient experience is now available for some alternative in vivo carcinogenicity models to support their application as complementary studies in combination with a single 2-yr carcinogenicity study to identify trans-species tumorigens. Our anal. of the rodent carcinogenicity studies supports such an approach for assessing carcinogenic potential without compromising the public health.

IT **108-46-3**, Resorcinol, biological studies **4342-03-4**
, Dacarbazine
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(rat and mouse carcinogenicity studies and evaluation of regulatory requirements for pharmaceuticals)

RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



RN 4342-03-4 HCAPLUS
CN 1H-Imidazole-4-carboxamide, 5-(3,3-dimethyl-1-triazenyl)- (9CI) (CA INDEX NAME)



CC 1-4 (Pharmacology)
IT 50-33-9, Phenylbutazone, biological studies 50-53-3, Chlorpromazine, biological studies 50-55-5, Reserpine 51-34-3, Scopolamine 52-53-9, Verapamil 53-86-1, Indomethacin 54-31-9, Furosemide 57-41-0, Phenytoin 57-66-9, Probenecid 57-68-1, Sulfamethazine 58-14-0, Pyrimethamine 58-25-3, Chlordiazepoxide 58-32-2, Dipyridamole 58-55-9, Theophylline, biological studies 58-73-1, Diphenhydramine 58-93-5, Hydrochlorothiazide 59-33-6 59-42-7, Phenylephrine 59-87-0, Nitrofurazone 60-54-8, Tetracycline 60-87-7, Promethazine 61-33-6, biological studies 64-77-7, Tolbutamide 67-20-9, Nitrofurantoin 67-45-8, Furazolidone 68-35-9, Sulfadiazine 69-53-4, Ampicillin 69-65-8, D-Mannitol 73-22-3, Tryptophan, biological studies 75-47-8, Iodoform 76-57-3, Codeine 77-09-8, Phenolphthalein 77-65-6, Carbromal 79-57-2, Oxytetracyclin 80-08-0 86-54-4, Hydralazine 91-64-5, Coumarin 94-20-2, Chlorpropamide 94-78-0, Phenazopyridine 97-53-0, Eugenol 98-96-4, Pyrazinamide 99-66-1, Valproic acid 103-90-2, Acetaminophen **108-46-3**, Resorcinol, biological studies 108-95-2, Phenol, biological studies 113-18-8, Ethchlorvinol 113-45-1, Methylphenidate 113-92-8 114-07-8, Erythromycin 114-86-3, Phenformin 115-77-5, biological studies 121-66-4, 2-Amino-5-nitrothiazole 127-69-5, Sulfisoxazole 128-13-2, Ursodeoxycholic acid 136-77-6, 4-Hexylresorcinol 139-94-6, Nithiazide 148-24-3, 8-Hydroxyquinoline, biological studies 148-79-8 299-42-3, Ephedrine 300-62-9, Amphetamine 303-53-7, Cyclobenzaprine 315-30-0, Allopurinol 389-08-2, Nalidixic acid 396-01-0, Triamterene 439-14-5, Diazepam 443-48-1, Metronidazole 486-12-4, Triprolidine 525-66-6, Propranolol 536-33-4, Ethionamide 554-10-9 555-30-6, Methyldopa 562-10-7 586-06-1, Metaproterenol 599-79-1, Sulfasalazine 604-75-1, Oxazepam 652-67-5, Isosorbide 671-16-9, Procarbazine 846-49-1, Lorazepam 846-50-4, Temazepam 968-81-0, Acetohexamide 1156-19-0, Tolazamide 1477-40-3, Levomethadyl acetate 1490-04-6, Menthol 1777-84-0 1972-08-3, Dronabinol 2062-78-4, Pimozide 2609-46-3, Amiloride 2955-38-6, Prazepam 3239-44-9, Dexfenfluramine 3385-03-3, Flunisolide 3771-19-5, Nafenopin 3930-20-9, Sotalol **4342-03-4**, Dacarbazine 4428-95-9, Foscarnet 5104-49-4, Flurbiprofen 5786-21-0, Clozapine 6493-05-6, Pentoxifylline 7261-97-4, Dantrolene 7488-56-4, Selenium sulfide 7681-49-4, Sodium fluoride, biological studies 9005-65-6, Polysorbate 80 10118-90-8, Minocycline 10238-21-8, Glyburide 10540-29-1, Tamoxifen 13292-46-1, Rifampin 13523-86-9, Pindolol 14769-73-4, Levamisole 15307-86-5, Diclofenac 15686-51-8, Clemastine 15722-48-2, Olsalazine 17560-51-9, MetolAzone 17617-23-1, Flurazepam 21256-18-8, Oxaprozin 22071-15-4,

Ketoprofen 22494-42-4, Diflunisal 22966-79-6, Estradiol mustard
23031-25-6, Terbutaline 24280-93-1, Mycophenolic acid
25451-15-4, Felbamate 25812-30-0, Gemfibrozil 26171-23-3,
Tolmetin 26308-28-1, Ripazepam 26807-65-8, Indapamide
26839-75-8, Timolol 27203-92-5, Tramadol 27591-01-1, Bunolol
29094-61-9, Glipizide 29110-47-2, Guanfacine 29122-68-7,
Atenolol 29975-16-4, Estazolam 30392-40-6, Bitolterol
30516-87-1, Zidovudine 31431-39-7, Mebendazole 31828-71-4,
Mexiletine 31883-05-3, Moricizine 34031-32-8, Auranofin
34911-55-2, Bupropion 36322-90-4, Piroxicam 36505-84-7,
Buspirone 36791-04-5, Ribavirin 36894-69-6, Labetalol
37517-30-9, Acebutolol 38363-40-5, Penbutolol 38677-81-5,
Pirbuterol 40391-99-9, Pamidronic acid 40580-59-4, Guanadrel
41340-25-4, Etodolac 41708-72-9, Tocainide 42200-33-9, Nadolol
42399-41-7, Diltiazem 42924-53-8, Nabumetone 50679-08-8,
Terfenadine 51333-22-3, Budesonide 51384-51-1, Metoprolol
51781-06-7, Carteolol 52645-53-1, Permethrin 53230-10-7,
Mefloquine 54063-35-3, Desogen 54063-53-5, Propafenone
54143-55-4, Flecainide 54182-58-0, Sucralfate 54350-48-0,
Etretinate 54910-89-3, Fluoxetine 55142-85-3, Ticlopidine
55985-32-5, Nicardipine 56211-40-6, Torsemide 56391-56-1,
Netilmicin 57801-81-7, Brotizolam 59122-46-2, Misoprostol
59277-89-3, Acyclovir 59467-70-8, Midazolam 59865-13-3,
Cyclosporine 60142-96-3, Gabapentin 60205-81-4, Ipratropium
60719-84-8, Amrinone 61869-08-7, Paroxetine 62571-86-2,
Captopril 63590-64-7, Terazosin 63659-18-7, Betaxolol
63675-72-9, Nisoldipine 64706-54-3, Bepridil 65277-42-1,
Ketoconazole 66085-59-4, Nimodipine 66104-22-1, Pergolide
66357-35-5, Ranitidine 66722-44-9, Bisoprolol 68844-77-9,
Astemizole 69049-73-6, Nedocromil 69655-05-6, Didanosine
72559-06-9, Rifabutin 73590-58-6, Omeprazole 74103-06-3,
Ketorolac 74191-85-8, Doxazosin 75330-75-5, Lovastatin
75695-93-1, Isradipine 75847-73-3, Enalapril 76824-35-6,
Famotidine 76963-41-2, Nizatidine 78415-72-2, Milrinone
79617-96-2, Sertraline 79794-75-5, Loratidine 79902-63-9,
Simvastatin 81093-37-0, Pravastatin 81098-60-4, Cisapride
82626-48-0, Zolpidem 83366-66-9, Nefazodone 83881-51-0,
Cetirizine 84057-84-1, Lamotrigine 84625-61-6, Itraconazole
85441-61-8, Quinapril 85721-33-1, Ciprofloxacin 86386-73-4,
Fluconazole 86541-75-5, Benazepril 87333-19-5 87848-99-5,
Acrivastine 88150-42-9, Amlodipine 91161-71-6, Terbinafine
93413-69-5, Venlafaxine 93957-54-1, Fluvastatin 98048-97-6,
Fosinopril 98319-26-7, Finasteride 99614-02-5, Ondansetron
103577-45-3, Lansoprazole 103628-46-2, Sumatriptan 104227-87-4,
Famciclovir 106266-06-2, Risperidone 109889-09-0, Granisetron
124832-26-4, Valacyclovir
RL: ADV (Adverse effect, including toxicity); BIOL (Biological
study)
(rat and mouse carcinogenicity studies and evaluation of
regulatory requirements for pharmaceuticals)

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

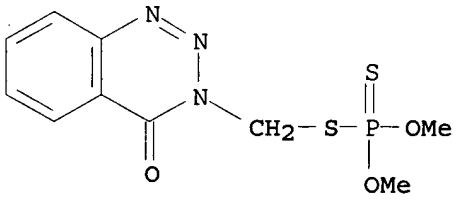
L67 ANSWER 11 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:662443 HCAPLUS
DOCUMENT NUMBER: 121:262443
TITLE: French limiting values for occupational exposure to chemicals
AUTHOR(S): Anon.

CORPORATE SOURCE: Fr.
SOURCE: Cahiers de Notes Documentaires (**1993**), 153, 557-74
CODEN: CNDIBJ; ISSN: 0007-9952
DOCUMENT TYPE: Journal
LANGUAGE: French

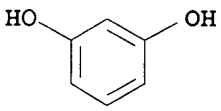
AB Limit values (suggested limiting values and max. permissible values) for occupational exposure to chems., including carcinogens, which have been published by the French Labor Ministry are presented in one table. This table is preceded by information on the following points: monitoring of workplace atmospheres (sampling and anal.; aerosols); permitted values (definitions and aims; additivity convention; elements and compds.; limiting occupational exposure values; carcinogens); mandatory values; and values recommended by the French National Health Insurance Fund (CNAM).

IT **86-50-0**, Azinphosmethyl **108-46-3**, Resorcinol, biological studies
RL: ADV (Adverse effect, including toxicity); POL (Pollutant); BIOL (Biological study); OCCU (Occurrence)
(occupational exposure; occupational exposure and stds. for limiting workplace concns. of chems. in France)

RN 86-50-0 HCAPLUS
CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



CC 59-5 (Air Pollution and Industrial Hygiene)

IT 50-00-0, Formaldehyde, biological studies 50-29-3, biological studies 54-11-5, Nicotine 55-63-0, Nitroglycerine 56-23-5, Tetrachloromethane, biological studies 56-38-2, Parathion 56-81-5, 1,2,3-Propanetriol, biological studies 57-14-7, 1,1-Dimethylhydrazine 57-24-9, Strychnine 57-50-1, biological studies 58-89-9, Lindane 60-29-7, biological studies 60-34-4, Methylhydrazine 60-57-1, Dieldrin 62-53-3, Aniline, biological studies 62-73-7, Dichlorvos 62-74-8 63-25-2, Carbaryl 64-17-5, Ethanol, biological studies 64-18-6, Formic acid, biological studies 64-19-7, Acetic acid, biological studies 67-56-1, Methanol, biological studies 67-63-0, Isopropanol, biological studies 67-64-1, Acetone, biological studies 67-66-3, Trichloromethane, biological studies 67-72-1, Hexachloroethane 68-11-1, Thioglycolic acid, biological studies 68-12-2, biological

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Methyl isobutyl ketone 108-11-2, 4-Methyl-2-pentanol 108-18-9,
Diisopropylamine 108-20-3, Diisopropyl ether 108-21-4, Isopropyl
acetate 108-24-7, Acetic anhydride 108-31-6, 2,5-Furandione,
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108-91-8, Cyclohexanamine, biological studies 108-93-0,
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108-98-5, Phenyl mercaptan, biological studies 109-59-1,
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biological studies 109-73-9, Butylamine, biological studies
109-79-5, Butanethiol 109-86-4, 2-Methoxyethanol 109-87-5,
Methylal 109-89-7, biological studies 109-94-4, Ethyl formate
109-99-9, biological studies 110-12-3, Methyl isoamyl ketone
110-19-0, Isobutyl acetate 110-43-0, 2-Heptanone 110-49-6,
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110-62-3, Valeraldehyde 110-80-5, 2-Ethoxyethanol 110-82-7,
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111-30-8, Pentanedial 111-40-0 111-42-2, Diethanolamine,
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Octane, biological studies 111-76-2, 2-Butoxyethanol 111-84-2,
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120-80-9, 1,2-Benzenediol, biological studies 120-82-1,
1,2,4-Trichlorobenzene 121-44-8, biological studies
RL: ADV (Adverse effect, including toxicity); POL (Pollutant); BIOL
(Biological study); OCCU (Occurrence)
(occupational exposure; occupational exposure and stds. for
limiting workplace concns. of chems. in France)

L67 ANSWER 12 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:200438 HCAPLUS
DOCUMENT NUMBER: 120:200438
TITLE: Controlled-release transdermal pharmaceuticals containing cryogels
INVENTOR(S): Wood, Louis L.; Calton, Gary J.
PATENT ASSIGNEE(S): SRCHEM Inc., USA

SOURCE: U.S., 15 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

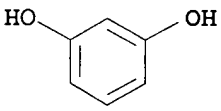
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5260066	A	19931109	US 1992-821627	19920116
US 5288503	A	19940222	US 1992-899369	19920616

PRIORITY APPLN. INFO.: US 1992-821627 A3 19920116

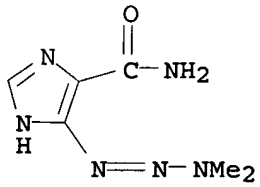
AB A controlled-release transdermal pharmaceutical contg. therapeutic agents in a poly(vinyl alc.) (I) cryogel is disclosed. A slurry of 11.0 mg ciprofloxacin.HCl (II) and 200 mg 10% I was warmed to 50-60° to obtain a clear homogeneous soln. The soln. was then placed in a mold and subjected to 6 freeze-thaw cycles to give a white opaque elastomeric cryogel having 15mm diam. and 0.5mm thickness. The release of II from the gel in 0.9% NaCl was 74% in th 1st 4 hs and it was const. in the subsequent 5-24 hs.

IT **108-46-3**, 1,3-Benzenediol, biological studies
4342-03-4, DTIC
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(controlled-release transdermal pharmaceuticals contg. cryogels and)

RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



RN 4342-03-4 HCAPLUS
CN 1H-Imidazole-4-carboxamide, 5-(3,3-dimethyl-1-triazenyl)- (9CI) (CA INDEX NAME)



IC ICM A61L015-16

INCL 424447000
CC 63-6 (Pharmaceuticals)
IT 50-00-0, Formaldehyde, biological studies 50-02-2, Dexamethasone 50-06-6, biological studies 50-07-7, Mitomycin C 50-18-0, Cytoxan 50-23-7, Hydrocortisone 50-24-8, Prednisolone 50-48-6, Amitriptyline 50-49-7, Imipramine 50-52-2, Thioridazine 50-53-3, Chlorpromazine, biological studies 50-56-6, Oxytocin, biological studies 50-76-0, Actinomycin D 50-78-2 50-81-7, Vitamin C, biological studies 51-05-8, Procaine hydrochloride 51-21-8, 5-Fluorouracil 51-34-3, Scopolamine 51-41-2, Levarterenol 51-43-4, Epinephrine 51-48-9, Thyroxine, biological studies 51-64-9, Dextroamphetamine 51-77-4, Gefarnate 52-53-9, Verapamil 52-86-8, Haloperidol 53-03-2, Prednisone 53-06-5, Cortisone 54-31-9, Furosemide 54-42-2, Idoxuridine 54-85-3, Isoniazide 54-91-1, Pipobroman 55-63-0 56-40-6, Glycine, biological studies 56-41-7, Alanine, biological studies 56-45-1, Serine, biological studies 56-54-2, Quinidine 56-75-7, Chloramphenicol 56-84-8, Aspartic acid, biological studies 56-85-9, Glutamine, biological studies 56-86-0, Glutamic acid, biological studies 56-87-1, Lysine, biological studies 57-27-2, Morphine, biological studies 57-41-0, Phenytoin 57-42-1, Meperidine 57-66-9, Probenecid 57-92-1, Streptomycin, biological studies 58-08-2, biological studies 58-14-0, Pyrimethamine 58-32-2, Dipyridamole 58-40-2, Promazine 58-54-8, Ethacrynic acid 58-55-9, Theophylline, biological studies 58-73-1, Diphenhydramine 58-74-2, Papaverine 58-93-5 59-01-8, Kanamycin 59-05-2, Methotrexate 59-33-6 59-46-1, Procaine 59-87-0 59-92-7, Levodopa, biological studies 60-54-8, Tetracycline 61-25-6, Papaverine hydrochloride 61-32-5, Methicillin 61-33-6, preparation 61-72-3, Cloxacillin 61-90-5, L-Leucine, biological studies 62-31-7, Dopamine hydrochloride 62-97-5, Diphemanil 63-68-3, Methionine, biological studies 63-91-2, Phenylalanine, biological studies 64-17-5, Ethanol, biological studies 65-49-6 66-79-5, Oxacillin 67-63-0, Isopropanol, biological studies 68-88-2, Hydroxyzine 69-23-8, Fluphenazine 69-43-2, Prenylamine lactate 69-53-4, Ampicillin 69-72-7, biological studies 70-00-8, Trifluridine 70-30-4, Hexachlorophene 71-00-1, Histidine, biological studies 72-19-5, Threonine, biological studies 72-44-6, Methaqualone 72-69-5 73-22-3, Tryptophan, biological studies 73-32-5, Isoleucine, biological studies 73-48-3 74-79-3, Arginine, biological studies 76-99-3, Methadone 77-07-6, Levorphanol 77-19-0, Dicyclomine 77-21-4, Glutethimide 78-11-5, Pentaerythritol tetranitrate 79-57-2, Oxytetracycline 81-23-2, Dehydrocholic acid 83-88-5, Vitamin G, biological studies 83-98-7, Orphenadrine 85-79-0, Dibucaine 86-21-5, Pheniramine 86-22-6, Brompheniramine 87-08-1, Penicillin V 87-33-2, Isosorbide dinitrate 90-82-4, Pseudoephedrine 91-81-6, Tripelennamine 94-09-7, Benzocaine 95-27-2, Dimazole 100-92-5, Mephentermine 101-31-5, Hyoscyamine **108-46-3**, 1,3-Benzenediol, biological studies 112-38-9, Undecylenic acid 113-15-5, Ergotamine 113-92-8 114-07-8, Erythromycin 115-38-8, Methylphenobarbital 118-23-0, Bromodiphenhydramine 118-42-3, Hydroxychloroquine 121-54-0 122-09-8, Phentermine 122-11-2, Sulfadimethoxine 125-29-1, Hydrocodone 125-71-3, Dextromethorphan 126-07-8, Griseofulvin 127-33-3, Demeclocycline 127-69-5, Sulfisoxazole 128-62-1, Noscapine 129-16-8, Mercurochrome 132-17-2 133-15-3 133-67-5, Trichlormethiazide 136-96-9 137-58-6, Lidocaine 144-80-9, Sulfacetamide 144-82-1, Sulfamethizole 147-24-0, Diphenhydramine hydrochloride 147-52-4, Nafcillin 147-85-3, Proline, biological studies 148-82-3,

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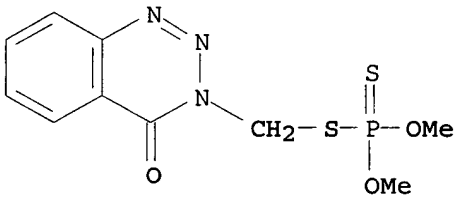
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(controlled-release transdermal pharmaceuticals contg. cryogels and)

L67 ANSWER 13 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:65829 HCAPLUS
DOCUMENT NUMBER: 118:65829
TITLE: Air contaminants
CORPORATE SOURCE: Occupational Safety and Health Administration, U. S. Dep. Labor, Washington, DC, 20210, USA
SOURCE: Federal Register (**1992**), 57(114, Bk. 2), 26002-601, 12 Jun 1992
CODEN: FEREAC; ISSN: 0097-6326
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Proposed amendments of existing air contaminant stds. for the maritime and construction industries and extension of air contaminant stds. to agricultural employees (only employees of farms with >10 nonfamily employees are covered) are given under the Federal Occupational Safety and Health Administration. Tables that indicated transitional limits, based on established threshold limit values, indication of skin protection needs, proposed time-weighted

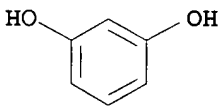
av. exposure (any 8-h work shift for 40-h week), short-term exposure limit (15-min time-weighted av.), ceiling (exposure during any part of the work day, or if instantaneous monitoring is not feasible, the 15-min time-weighted av.), and/or skin protection needs are given for the shipyard, marine terminal and longshoring, construction, and agricultural industries. Extensive data on health effects of the substances to be regulated and preliminary regulatory impact analyses are given for general industry and the specific industrial sectors.

IT **86-50-0**, Azinphos-methyl **108-46-3**, Resorcinol, biological studies
RL: ADV (Adverse effect, including toxicity); POL (Pollutant); BIOL (Biological study); OCCU (Occurrence)
(exposure limits to airborne, in agricultural and construction and maritime industries, stds. for)

RN 86-50-0 HCAPLUS
CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



CC 59-5 (Air Pollution and Industrial Hygiene)

IT 50-00-0, Formaldehyde, biological studies 50-29-3, DDT, miscellaneous 50-78-2, Acetylsalicylic acid 54-11-5, Nicotine 55-38-9, Fenthion 55-63-0, Nitroglycerin 56-23-5, Carbon tetrachloride, biological studies 56-38-2, Parathion 56-81-5, 1,2,3-Propanetriol, biological studies 57-14-7, 1,1-Dimethylhydrazine 57-24-9, Strychnine 57-50-1, Sucrose, biological studies 57-57-8, 2-Oxetanone 58-89-9, Lindane 60-29-7, Ethyl ether, biological studies 60-34-4, Methyl hydrazine 60-57-1, Dieldrin 61-82-5, Amitrole 62-53-3, Aniline, biological studies 62-53-3D, Aniline, homologs 62-73-7, Dichlorvos 62-74-8 62-75-9, N-Nitrosodimethylamine 63-25-2 64-17-5, Ethyl alcohol, biological studies 64-18-6, Formic acid, biological studies 64-19-7, Acetic acid, biological studies 67-56-1, Methyl alcohol, biological studies 67-63-0, 2-Propanol, biological studies 67-64-1, Acetone, biological studies 67-66-3, Chloroform, biological studies 67-72-1, Hexachloroethane 68-11-1, Thioglycolic acid, biological studies 68-12-2, Dimethylformamide, biological studies 71-23-8, n-Propyl alcohol, biological studies 71-43-2, Benzene, biological studies 71-55-6, Methyl chloroform 72-20-8, Endrin 72-43-5 74-83-9, Methyl

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RL: ADV (Adverse effect, including toxicity); POL (Pollutant); BIOL (Biological study); OCCU (Occurrence)
(exposure limits to airborne, in agricultural and construction and maritime industries, stds. for)

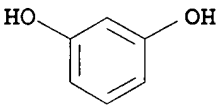
L67 ANSWER 14 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:628214 HCAPLUS
DOCUMENT NUMBER: 117:228214
TITLE: Structural basis of the in vivo induction of micronuclei
AUTHOR(S): Yang, Wu Lung; Klopman, Gilles; Rosenkranz, Herbert S.
CORPORATE SOURCE: Grad. Sch. Public Health, Univ. Pittsburgh, Pittsburgh, PA, 15261, USA
SOURCE: Mutation Research (**1992**), 272(2), 111-24
CODEN: MUREAV; ISSN: 0027-5107

DOCUMENT TYPE: Journal
LANGUAGE: English

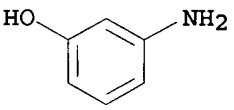
AB The structural basis of the in vivo induction of micronuclei was examd. with CASE, a structure-activity relational method. The CASE program identified a no. of structures assocd. with this activity. When used to predict the activity of chems. not included in the learning set, these structural determinants gave a concordance in excess of 83%. The existence of a structural basis for the induction of micronuclei will permit an investigation of the mechanistic basis of this phenomenon.

IT **108-46-3**, 1,3-Benzenediol, properties **591-27-5**
7203-90-9 7227-91-0, 3,3-Dimethyl-1-phenyltriazene
7239-21-6 50355-74-3
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(micronuclei induction by, structural basis of, evaluation of)

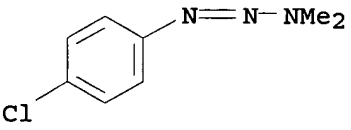
RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



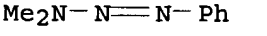
RN 591-27-5 HCAPLUS
CN Phenol, 3-amino- (9CI) (CA INDEX NAME)



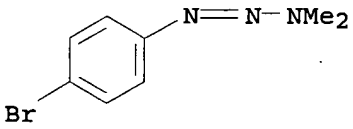
RN 7203-90-9 HCAPLUS
CN 1-Triazene, 1-(4-chlorophenyl)-3,3-dimethyl- (9CI) (CA INDEX NAME)



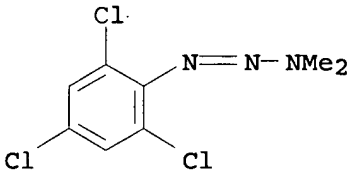
RN 7227-91-0 HCAPLUS
CN 1-Triazene, 3,3-dimethyl-1-phenyl- (9CI) (CA INDEX NAME)



RN 7239-21-6 HCAPLUS
CN 1-Triazene, 1-(4-bromophenyl)-3,3-dimethyl- (9CI) (CA INDEX NAME)



RN 50355-74-3 HCAPLUS
CN 1-Triazene, 3,3-dimethyl-1-(2,4,6-trichlorophenyl)- (9CI) (CA INDEX NAME)



CC 4-6 (Toxicology)
IT 50-00-0, Formaldehyde, biological studies 50-06-6, Phenobarbital, biological studies 50-07-7, Mitomycin C 50-18-0, Cyclophosphamide 50-21-5, Lactic acid, biological studies 50-29-3, properties 50-32-8, Benzo(a)pyrene, biological studies 50-33-9, Phenylbutazone, biological studies 50-37-3 50-41-9 50-44-2, 6-Mercaptopurine 50-69-1, Ribose 50-76-0, Actinomycin D 50-78-2 50-81-7, L-Ascorbic acid, biological studies 50-91-9, 5-Fluorodeoxyuridine 50-99-7, D-Glucose, biological studies 51-02-5 51-18-3, Triethylenemelamine 51-21-8, 5-Fluorouracil 51-43-4 51-61-6, Dopamine, biological studies 51-75-2, Mechlorethamine 51-79-6, Urethane 52-24-4, Thio-tepa 52-28-8 52-68-6 52-90-4, Cysteine, biological studies 53-86-1, Indomethacin 53-96-3, 2-Acetylaminofluorene 54-42-2 54-62-6, Aminopterin 55-18-5 55-21-0, Benzamide 55-98-1, Busulfan 56-40-6, Glycine, biological studies 56-41-7, Alanine, biological studies 56-49-5 56-53-1 56-57-5, 4-Nitroquinoline N-oxide 56-81-5, 1,2,3-Propanetriol, biological studies 56-82-6, Glyceraldehyde 56-84-8, Aspartic acid, biological studies 56-86-0, Glutamic acid, biological studies 57-00-1, Creatine 57-13-6, Urea, biological studies 57-14-7 57-15-8 57-22-7, Vincristine 57-39-6, Metepa 57-41-0 57-50-1, biological studies 57-57-8, 2-Oxetanone 57-87-4, Ergosterol 57-88-5, Cholesterol, biological studies 57-97-6, 7,12-Dimethylbenz(a)-anthracene 58-08-2, biological studies 58-85-5, Biotin 59-02-9, α-Tocopherol 59-05-2, Methotrexate 59-14-3, 5-Bromo-2'-deoxyuridine 59-67-6, Niacin, biological studies 59-87-0 59-89-2, N-Nitrosomorpholine 60-11-7, 4-Dimethylaminoazobenzene 60-18-4, L-Tyrosine, biological studies 60-35-5, Acetamide, biological studies 60-51-5 60-56-0 61-82-5, 1H-1,2,4-Triazol-3-amine 61-90-5, Leucine, biological studies 62-44-2, Phenacetin 62-49-7 62-50-0, Ethyl methanesulfonate 62-53-3, Benzenamine, biological studies 62-55-5, Thioacetamide 62-73-7 62-75-9, Dimethylnitrosamine 63-25-2 63-42-3, Lactose 63-68-3, L-Methionine, biological studies 63-75-2, Arecoline 63-91-2, Phenylalanine, biological studies 64-17-5, Ethanol, biological studies 64-77-7, Tolbutamide 64-86-8, Colchicine 65-61-2, Acridine orange 66-27-3, Methyl methanesulfonate 66-81-9, Cycloheximide 67-20-9,

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298-00-0, Methyl parathion 298-02-2, Phorate 298-12-4, Glyoxylic acid 300-62-9, Amphetamine
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(micronuclei induction by, structural basis of, evaluation of)

IT 301-12-2, Oxydemeton-methyl 302-17-0 303-33-3, Heliotrine 303-34-4 305-03-3, Chlorambucil 306-37-6, 1,2-Dimethylhydrazine dihydrochloride 309-00-2 328-42-7, Oxaloacetic acid 331-39-5 353-59-3, Bromochlorodifluoromethane 372-75-8, Citrulline 404-86-4, Capsaicin 438-41-5 439-14-5 443-48-1, Metronidazole 446-86-6, Azathioprine 451-13-8, Homogentisic acid 476-28-8 477-30-5, Colcemid 482-89-3 495-48-7, Azoxybenzene 496-72-0, 4-Methyl-o-phenylenediamine 499-04-7 506-26-3 506-32-1 512-56-1, Trimethyl phosphate 520-18-3, Kaempferol 520-52-5 521-35-7, Cannabinol 522-40-7 525-66-6, Propranolol 526-95-4, D-Gluconic acid 540-73-8 541-15-1, Carnitine 541-50-4, Acetoacetic acid, biological studies 541-73-1 547-58-0 548-83-4, Galangin 589-41-3, N-Hydroxyurethane **591-27-5** 604-59-1 615-05-4 622-97-9 624-83-9, Methyl isocyanate 630-93-3, 5,5-Diphenylhydantoin sodium 632-24-6 636-21-5 671-16-9, Procarbazine 680-31-9, Hexamethylphosphoramide, biological studies 759-73-9 781-43-1 865-21-4, Vinblastine 924-16-3 926-06-7, Isopropyl methanesulfonate 959-24-0 1068-57-1 1070-11-7, Ethambutol hydrochloride 1116-54-7 1143-38-0 1197-19-9 1667-11-4, 4-Chloromethylbiphenyl 1684-42-0, Acranil hydrochloride 1689-89-0 1746-01-6 1836-75-5 1836-77-7 1934-21-0 1953-02-2 1972-08-3 2055-46-1 2227-79-4, Thiobenzamide 2277-92-1 2353-45-9, Fast green FCF 2426-08-6, Glycidyl-n-butyl ether 2465-27-2 2682-20-4, 2-Methyl-3-isothiazolone 2835-96-3 3148-73-0 3171-45-7 3380-34-5 3416-24-8, Glucosamine 3544-94-3 3597-91-9, 4-Hydroxymethylbiphenyl 3688-53-7 3710-84-7 3715-92-2 3778-73-2, Ifosfamide 4719-04-4 4803-27-4 5307-14-2 5348-42-5 6369-59-1 6452-71-7, Oxprenolol 6673-35-4 6804-07-5, Carbadox 6915-15-7 6923-22-4, Monocrotophos **7203-90-9 7227-91-0**, 3,3-Dimethyl-1-phenyltriazene 7235-40-7, β,β-Carotene **7239-21-6** 7681-76-7 7790-92-3, Hypochlorous acid 10034-93-2 10238-21-8 10599-90-3, Chloramide 11103-57-4, Vitamin A 12684-33-2, Sibiromycin 13073-35-3, Ethionine 13171-21-6, Phosphamidon 13523-86-9 13956-29-1, Cannabidiol 14073-00-8, 3-Methyl-4-nitro-quinoline N-oxide 15263-53-3 16423-68-0, Erythrosine 20702-77-6, Neohesperidin dihydrochalcone 21739-91-3, Cytembena 22089-22-1, Trofosfamide 22994-85-0, Benznidazole 23049-93-6 23214-92-8, Adriamycin 23255-93-8, Hycanthone methanesulfonate 23256-30-6, Nifurtimox 23696-28-8, Olaquindox 24632-47-1, Nifurpipone 26172-55-4 28322-02-3 29122-68-7 29868-97-1 30560-19-1 35050-55-6 35367-38-5 37753-10-9, Sufosfamide **50355-74-3** 51264-14-3, m-AMSA 51384-51-1 52315-07-8, Cypermethrin 54063-53-5 54350-48-0 54827-17-7, 3,3',5,5'-Tetramethyl-benzidine 57808-66-9, Domperidone 59865-13-3, Cyclosporin A 63358-49-6 65009-35-0 65589-70-0, Acriflavine 68844-77-9 69866-21-3, Rachelmycin 71031-15-7, Cathinone 76180-96-6, IQ
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(micronuclei induction by, structural basis of, evaluation of)

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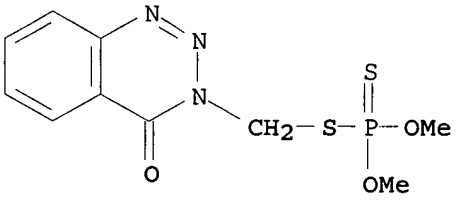
ACCESSION NUMBER: 1992:402498 HCAPLUS
DOCUMENT NUMBER: 117:2498

TITLE: A QSAR model of teratogenesis
AUTHOR(S): Gombar, Vijay K.; Borgstedt, Harold H.; Enslein, Kurt; Hart, Jeffrey B.; Blake, Benjamin W.
CORPORATE SOURCE: Health Des., Inc., Rochester, NY, 14604, USA
SOURCE: Quantitative Structure-Activity Relationships (**1991**), 10(4), 306-32
CODEN: QSARDI; ISSN: 0931-8771
DOCUMENT TYPE: Journal
LANGUAGE: English

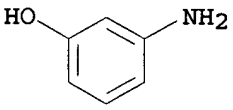
AB Four related QSAR models of teratogenesis in exptl. animals have been developed: one each for heteroarom., carboarom., alicyclic and acyclic compds. The nos. of compds. in these models range from 40 (for the alicyclic model) to 144 (for the carboarom. model). As detd. by cross-validation using the leave-one-out, or jackknife, technique, the accuracy of the models in discriminating between teratogens and nonteratogens ranges from 92.4% to 96%. A single overall assessment of exptl. teratogenesis was chosen as the biol. endpoint; taking into account such factors as dosage, maternal toxicity, and affected organ systems remain to be subjects of further studies.

IT **86-50-0**, Azinphos-Methyl **591-27-5**
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(teratogenesis in lab. animals from, QSAR model of)

RN 86-50-0 HCAPLUS
CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



RN 591-27-5 HCAPLUS
CN Phenol, 3-amino- (9CI) (CA INDEX NAME)



CC 4-6 (Toxicology)
Section cross-reference(s): 1

IT 50-36-2, Cocaine 50-49-7, Imipramine 51-12-7, Nialamide 52-67-5, Penicillamine 52-68-6, Dipterex 53-86-1, Indomethacin 54-32-0, Moxisylyte 55-38-9, Fenthion 55-63-0, Nitroglycerin 56-87-1, Lysine, biological studies 57-13-6, Urea, biological studies 57-41-0, Phenytoin 57-44-3 58-08-2, Caffeine, biological studies 58-14-0, 2,4-Diamino-5-p-chlorophenyl-6-ethyl-pyrimidine 58-25-3, Chlordiazepoxide 58-55-9, Theophylline, biological studies 58-73-1, Diphenhydramine 58-89-9, Lindane 58-90-2, 2,3,4,6-Tetrachlorophenol 58-94-6, Chlorothiazide 59-14-3, 5-Bromodeoxyuridine 59-66-5, Acetazolamide 60-00-4,

biological studies 60-57-1, Dieldrin 62-53-3, Aniline, biological studies 62-56-6, Thiourea, biological studies 62-73-7, Dichlorvos 63-25-2, Carbaryl 64-17-5, Ethanol, biological studies 64-86-8, Colchicine 67-20-9, Nitrofurantoin 67-56-1, Methanol, biological studies 67-66-3, Chloroform, biological studies 70-30-4, Hexachlorophene 71-43-2, Benzene, biological studies 71-55-6, 1,1,1-Trichloroethane 72-20-8, Endrin 72-55-9, 1,1-Dichloro-2,2-bis(p-chloro-phenyl)-ethylene, biological studies 73-22-3, L-Tryptophan, biological studies 75-01-4, Vinyl chloride, biological studies 75-05-8, Acetonitrile, biological studies 75-07-0, Acetaldehyde, biological studies 75-09-2, Methylene chloride, biological studies 75-21-8, Ethylene oxide, biological studies 75-35-4, Vinylidene chloride, biological studies 77-47-4, Hexachlorocyclopentadiene 78-30-8, Tri-o-cresyl phosphate 79-06-1, Acrylamide, biological studies 80-05-7, Bisphenol A, biological studies 82-93-9, Chlorcyclizine 83-67-0, Theobromine 83-79-4, Rotenone 84-74-2, Dibutylphthalate 85-73-4 **86-50-0**, Azinphos-Methyl 87-86-5, Pentachlorophenol; 90-43-7, 2-Phenylphenol 91-20-3, Naphthalene, biological studies 92-52-4, Biphenyl, biological studies 93-76-5, (2,4,5-Trichlorophenoxy)-acetic acid 95-50-1, o-Dichlorobenzene 95-55-6, o-Aminophenol 95-94-3, 1,2,4,5-Tetrachlorobenzene 96-09-3, Styrene oxide 96-12-8, 1,2-Dibromo-3-chloropropane 96-45-7, Ethylenethiourea 97-77-8, Disulfiram 98-95-3, Nitrobenzene, biological studies 99-56-9, 4-Nitro-o-Phenylenediamine 99-66-1 99-98-9, N,N-Dimethyl-p-phenylenediamine 100-42-5, Styrene, biological studies 100-44-7, Benzyl chloride, biological studies 106-46-7, p-Dichlorobenzene 106-50-3, p-Phenylenediamine, biological studies 106-89-8, Epichlorohydrin, biological studies 106-93-4, Ethylene dibromide 107-05-1, Allyl chloride 107-06-2, 1,2-Dichloroethane, biological studies 107-12-0, Propionitrile 107-21-1, Ethylene glycol, biological studies 107-35-7, Taurine 108-10-1, Methylisobutyl ketone 108-88-3, Toluene, biological studies 108-90-7, Monochlorobenzene, biological studies 109-79-5, n-Butylmercaptan 109-86-4, Ethylene glycol monomethyl ether 110-61-2, Succinonitrile 110-80-5, Ethylene glycol monoethyl ether 111-15-9, Ethylene glycol monoethyl ether acetate 111-46-6, Diethylene glycol, biological studies 111-69-3, Adiponitrile 111-76-2, Ethylene glycol monobutyl ether 111-94-4 111-96-6, Diethylene glycol dimethyl ether 112-24-3, Triethylenetetramine 112-34-5, Diethylene glycol monobutyl ether 112-49-2, Triethylene glycol dimethyl ether 117-81-7, Di-(2-EThylhexyl)-phthalate 120-72-9, Indole, biological studies 121-14-2, 2,4-Dinitrotoluene 121-45-9, Trimethyl phosphite 122-99-6, Ethylene glycol monophenyl ether 123-30-8, p-Aminophenol 123-91-1, Dioxane, biological studies 126-72-7, Tris-(2,3-dibromopropyl)-phosphate 133-06-2, Captan 137-58-6, Lidocaine 140-88-5, Ethyl acrylate 141-32-2 142-28-9, 1,3-Dichloropropane 148-79-8, Thiabendazole 154-23-4, Cianidanol 154-93-8, N,N'-Bis-(2-chloroethyl)-N-nitrosourea 299-84-3 302-17-0, Chloral hydrate 303-33-3, Heliotrine 303-45-7, Gossypol 303-47-9, Ochratoxin A 309-00-2, Aldrin 329-89-5, 6-Aminonicotinamide 330-55-2, Linuron 362-74-3 363-24-6 437-38-7, Fentanyl 474-25-9, Chenodeoxycholic acid 525-66-6 530-78-9, Flufenamic acid 537-46-2, Methamphetamine 554-35-8, Linamarin 586-06-1 **591-27-5** 598-50-5, 1-Methylurea 598-52-7, 1-Methylthiourea 608-25-3, 2-Methyl Resorcinol 615-66-7, 2-Chloro-1,4-benzenediamine 625-52-5, 1-Ethylurea 625-53-6, 1-Ethylthiourea 632-21-3, 1,1,3,3-Tetrachloroacetone 634-66-2, 1,2,3,4-Tetrachlorobenzene

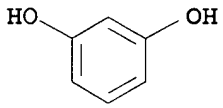
634-90-2, 1,2,3,5-Tetrachlorobenzene 642-72-8 644-62-2
645-05-6, Hexamethylmelamine 671-16-9, Procarbazine 684-16-2
695-53-4, Dimethadione 732-11-6, Imidan 745-65-3, Prostaglandin
E-1 764-41-0, 1,4-Dichloro-2-butene 804-30-8, Thiamine
tetrahydrofurfuryl disulfide 872-50-4, biological studies
897-15-4, Dosulepin chloride 1622-62-4, Flunitrazepam 1634-04-4,
Methyl-tert-butyl ether 1702-17-6, 3,6-Dichloropicolinic acid
1746-01-6, 2,3,7,8-Tetrachlorodibenzo-p-Dioxin 1812-30-2,
Bromazepam 1825-21-4 1836-75-5, 2,4-Dichlorophenyl-p-Nitrophenyl
ether 1918-02-1, Picloram 1934-21-0, Tartrazine 1948-33-0,
tert-Butylhydroquinone 1972-08-3 2062-78-4, Pimozide 2310-17-0
2321-07-5 2698-38-6, 4-Chloro-2-methylphenoxyaceticacid ethyl
ester 2698-41-1, o-Chlorobenzylidene malononitrile 2809-21-4
2921-88-2, Chlorpyrifos 2955-38-6, Prazepam 3385-03-3,
Flunisolide 3562-84-3, Benzbromarone 3715-92-2,
N-Nitrosoethylenethiourea 3778-73-2, Ifosfamide 3825-26-1,
Ammonium perfluorooctanoate 4376-20-9, Mono(2-Ethylhexyl)phthalate
4559-86-8, 1,1,3,3-Tetrabutylurea 5051-62-7, Guanabenz
5307-14-2, 2-Nitro-p-phenylenediamine 5464-28-8,
1,3-Dioxolane-4-methanol 5534-09-8 5633-20-5, Oxybutynin
6051-87-2, β-Naphthoflavone 6358-09-4, 6-Chloro-4-nitro-2-
aminophenol 6493-05-6, Pentoxifylline 6837-24-7,
N-Cyclohexyl-2-pyrrolidone 6903-79-3, Creatinol-o-phosphate
7235-40-7, β-Carotene 9036-19-5, Octoxynol 10206-21-0,
Cephacetrile 10457-90-6, Bromperidol 10540-29-1, Tamoxifen
11121-48-5, Rose bengal 13392-18-2, Fenoterol 13993-65-2,
Metiazinic acid 14255-87-9, Parbendazole 14769-73-4, Levamisole
15687-27-1, Ibuprofen 17804-35-2, Benomyl 17924-92-4,
Zearalenone 18046-21-4, Fentiazac 18172-33-3, Cyclopiazonic acid
18683-91-5, Ambroxol 19216-56-9, Prazosin 19875-60-6, Lisuride
hydrogen maleate 20537-88-6, Amifostine 20706-25-6 21187-98-4
21256-18-8, Oxaprozin 21259-20-1, Insariotoxin 21466-07-9,
Bromofenofos 21609-90-5, Phosvel 21794-01-4, Rubratoxin B
22059-60-5, Disopyramide phosphate 22316-47-8, Clobazam
22345-47-7, Tofisopam 22494-42-4, Diflunisal 22609-73-0,
Niludipine 23155-02-4, Fosfomycin 23210-56-2, Ifenprodil
23255-93-8, Hycanthone methane sulfonate 23256-30-6, Nifurtimox
24729-96-2, Clindamycin 2-phosphate 25122-57-0, Clobetasone
17-butyrate 25967-29-7, Flutoprazepam 26328-04-1, Cinepazide
maleate 26615-21-4, Zotepine 26652-09-5, Ritodrine 26675-46-7,
Isoflurane 26807-65-8, Indapamide 26864-56-2 27470-51-5,
Suxibuzone 27589-33-9, Azosemide 28657-80-9, Cinoxacin
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL
(Biological study)
(teratogenesis in lab. animals from, QSAR model of)

L67 ANSWER 16 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:116537 HCAPLUS
DOCUMENT NUMBER: 114:116537
TITLE: Interactions of halogenated industrial chemicals with transthyretin and effects on thyroid hormone levels in vivo
AUTHOR(S): Van den Berg, K. J.; Van Raaij, J. A. G. M.; Bragt, P. C.; Notten, W. R. F.
CORPORATE SOURCE: TNO Med. Biol. Lab., Rijswijk, 2280 AA, Neth.
SOURCE: Archives of Toxicology (**1991**), 65(1), 15-19
CODEN: ARTODN; ISSN: 0340-5761
DOCUMENT TYPE: Journal
LANGUAGE: English

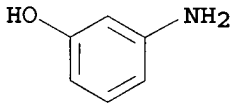
AB Some 65 compds. from 12 chem. groups were analyzed for direct interference with the T4 binding site of transthyretin using a competitive binding assay. Sixty per cent of the compds. were competitive at 100 μM. Relatively strong interactions were obsd. by several chlorophenols, chlorophenoxy acids, and nitrophenols, as well as by individual compds. such as hexachlorobenzene, dicofol, bromoxynil, and tetrachlorohydroquinone. Examples from these chem. groups, e.g., pentachlorophenol, 2,4-dichlorophenoxybutyric acid, dinoseb, and bromoxynil, also reduced plasma T4 levels in rats. In addn., bromoxynil decreased plasma T3 levels. The results suggest the existence of a no. of halogenated industrial chems. with a potential for lowering plasma thyroid hormone levels through interference with hormone transport carriers.

IT **108-46-3**, Resorcinol, biological studies **591-27-5**, 3-Aminophenol **2642-71-9**, Ethyl-azinphos
RL: BIOL (Biological study)
(thyroid hormone response and transthyretin interaction to)

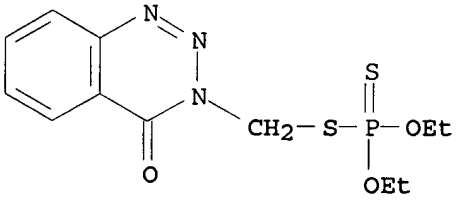
RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



RN 591-27-5 HCAPLUS
CN Phenol, 3-amino- (9CI) (CA INDEX NAME)



RN 2642-71-9 HCAPLUS
CN Phosphorodithioic acid, O,O-diethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



CC 4-3 (Toxicology)

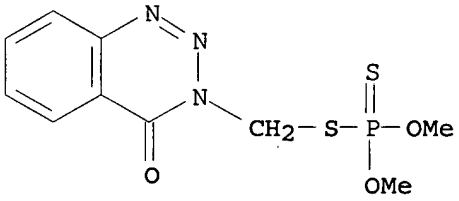
IT 50-29-3D, DDT, derivs 51-28-5, 2,4-Dinitrophenol, biological studies 53-19-0, o,p'-DDD 56-23-5, Tetrachloromethane, biological studies 56-38-2, Ethyl-parathion 58-89-9, Hexachlorocyclohexane 67-66-3, Chloroform, biological studies 67-72-1, Hexachloroethane 70-30-4, Hexachlorophene 71-43-2, Benzene, biological studies 71-43-2D, Benzene, chloro derivs. 72-43-5, Methoxychlor 72-54-8, DDD 76-03-9, Trichloroacetic acid, biological studies 79-01-6, Trichloroethylene, biological

studies 87-65-0, 2,6-Dichlorophenol 87-66-1, Pyrogallol 87-86-5, Pentachlorophenol 87-87-6 88-06-2, 2,4,6-Trichlorophenol 88-85-7, Dinoseb 90-43-7, 2-Hydroxybiphenyl 92-52-4D, Biphenyl, derivs. 92-69-3, 4-Hydroxybiphenyl 93-72-1, Fenoprop 93-76-5, 2,4,5-Trichlorophenoxyacetic acid 94-74-6, MCPA 94-75-7, 2,4-D, biological studies 94-81-5, MCPB 94-82-6, 2,4-DB 95-48-7, o-Cresol, biological studies 95-57-8, 2-Chlorophenol 95-95-4, 2,4,5-Trichlorophenol 98-54-4, 4-tert-Butylphenol 101-42-8D, derivs. 106-48-9, 4-Chlorophenol 108-43-0, 3-Chlorophenol **108-46-3**, Resorcinol, biological studies 108-95-2, Phenol, biological studies 108-95-2D, Phenol, chloro and nitro derivs. 115-29-7, Endosulfan 115-32-2 117-81-7 118-74-1, Hexachlorobenzene 120-36-5, Dichloroprop 120-80-9, Catechol, biological studies 120-83-2, 2,4-Dichlorophenol 121-75-5, Malathion 127-18-4, Perchloroethylene, biological studies 128-37-0, 2,6-Di-tert-butyl-4-methylphenol, biological studies 150-68-5, Monuron 302-17-0, Chloral hydrate 311-45-5 330-54-1, Diuron 330-55-2, Linuron 534-52-1, DNOC 555-37-3, Neburon 576-24-9, 2,3-Dichlorophenol **591-27-5**, 3-Aminophenol 997-50-2D, derivs. 1631-73-8D, derivs. 1689-84-5 1928-37-6, 2,4,5-Trichlorophenoxyacetic acid methyl ester 1982-47-4, Chloroxuron **2642-71-9**, Ethyl-azinphos 4824-78-6, Ethyl-bromophos 7723-14-0D, Phosphorus, org. compds. 12002-48-1, Trichlorobenzene 25321-22-6, Dichlorobenzene 25322-20-7, Tetrachloroethane 32598-13-3, 3,4,3',4'-Tetrachlorobiphenyl
RL: BIOL (Biological study)
(thyroid hormone response and transthyretin interaction to)

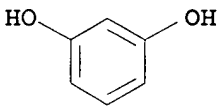
L67 ANSWER 17 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:173827 HCAPLUS
DOCUMENT NUMBER: 112:173827
TITLE: The structural basis of the mutagenicity of chemicals in Salmonella typhimurium: The Gene-Tox data base
AUTHOR(S): Klopman, Gilles; Frierson, Manton R.; Rosenkranz, Herbert S.
CORPORATE SOURCE: Dep. Chem., Case West. Reserve Univ., Cleveland, OH, 44106, USA
SOURCE: Mutation Research (**1990**), 228(1), 1-50
CODEN: MUREAV; ISSN: 0027-5107
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The CASE (Computer Automated Structure Evaluation) structure-activity methodol. has been applied to a Gene-Tox derived Salmonella mutagenicity data base consisting of 808 chems. Based upon qual. structural features, CASE identified 29 activating and 3 inactivating structural determinants which correctly predicted the probability of carcinogenicity of 93.7% of the known mutagens and nonmutagens in the data base (sensitivity = 0.998, and specificity = 0.704). Addnl., based upon a qual. structure-activity anal., CASE's performance was even better, leading to a sensitivity of 0.981 and a specificity of 1.000. Using the structural determinants identified in this data base, CASE gave excellent predictions of the mutagenicity of chems. not included in the data base. The identified biophores and biophobes can also be used to investigate the structural basis of the mutagenicity of various chem. classes.
IT **86-50-0**, Azinphos-methyl **108-46-3**, Resorcinol, biological studies **150-70-9**
RL: ADV (Adverse effect, including toxicity); BIOL (Biological

study)
(mutagenicity of, Computer Automated Structure Evaluation for study of structural determinants in relation to)

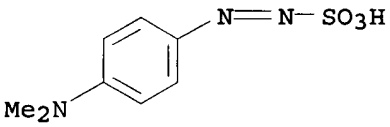
RN 86-50-0 HCAPLUS
CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



RN 150-70-9 HCAPLUS
CN Diazenesulfonic acid, [4-(dimethylamino)phenyl]- (9CI) (CA INDEX NAME)



CC 4-6 (Toxicology)
Section cross-reference(s): 1, 5, 20

IT 50-06-6, Phenobarbital, biological studies 50-07-7, Mitomycin C 50-18-0, Cyclophosphamide 50-29-3, biological studies 50-32-8, Benzo[a]pyrene, biological studies 50-33-9, Phenylbutazone, biological studies 50-44-2, 6-Mercaptopurine 50-81-7, L-Ascorbic acid, biological studies 51-21-8, 5-Fluorouracil 51-34-3, Scopolamine 51-55-8, Atropine, biological studies 51-79-6, Urethane 52-24-4, Thio-TEPA 52-68-6, Trichlorfon 53-70-3, Dibenz[a,h]anthracene 53-94-1, N-Hydroxy-2-aminofluorene 53-95-2, N-Hydroxy-2-acetylaminofluorene 53-96-3 54-11-5, Nicotine 54-31-9, Furosemide 54-42-2, 5-Iododeoxyuridine 54-88-6 55-18-5, Diethylnitrosamine 55-38-9, Fenthion 55-86-7, Nitrogen mustard 56-23-5, Carbon tetrachloride, biological studies 56-38-2, Ethyl parathion 56-49-5, 3-Methylcholanthrene 56-53-1, Diethylstilbestrol 56-55-3, Benz[a]anthracene 56-57-5, 4-Nitroquinoline-1-oxide 56-75-7, Chloramphenicol 57-14-7, 1,1-Dimethylhydrazine 57-57-8, β-Propiolactone 57-67-0, Sulfaguanidine 57-94-3 57-97-6 58-08-2, biological studies 58-14-0 58-25-3, Chlordiazepoxide 58-93-5, Hydrochlorothiazide 58-94-6, Chlorothiazide 59-05-2, Methotrexate 59-46-1 59-87-0,

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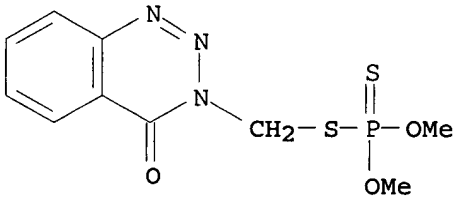
p-Nitroanisole 100-32-3, Bis(4-nitrophenyl) disulfide 100-42-5, biological studies 100-44-7, Benzyl chloride, biological studies 100-75-4, N-Nitrosopiperidine 101-14-4 101-54-2, N-Phenyl-p-phenylenediamine 103-30-0, trans-Stilbene 103-33-3, Azobenzene 103-84-4, Acetanilide 103-90-2 106-88-7, 1,2-Epoxybutane 106-89-8, biological studies 106-93-4, 1,2-Dibromoethane 107-06-2, 1,2-Dichloroethane, biological studies 107-07-3, Ethylene chlorohydrin, biological studies 107-13-1, 2-Propenenitrile, biological studies 107-20-0, 2-Chloroacetaldehyde 107-21-1, 1,2-Ethanediol, biological studies 108-05-4, Acetic acid ethenyl ester, biological studies 108-30-5, Succinic anhydride, biological studies 108-45-2, m-Phenylenediamine, biological studies **108-46-3**, Resorcinol, biological studies 108-86-1, Bromobenzene, biological studies 109-84-2, N-(2-Hydroxyethyl)hydrazine 110-82-7, Cyclohexane, biological studies 115-02-6, Azaserine 115-20-8, 2,2,2-Trichloroethanol 115-90-2, Fensulfothion 116-63-2 116-83-6, 1-Amino-4-methoxyanthraquinone 116-85-8 117-39-5, Quercetin 117-62-4 118-96-7, 2,4,6-Trinitrotoluene 119-26-6, 2,4-Dinitrophenylhydrazine 119-27-7, 2,4-Dinitroanisole 119-65-3, Isoquinoline 119-90-4, 3,3'-Dimethoxybenzidine 120-12-7, Anthracene, biological studies 120-58-1, Isosafrole 121-75-5, Malathion 121-88-0, 2-Amino-5-nitrophenol 121-92-6, 3-Nitrobenzoic acid 122-34-9, Simazine 123-30-8 123-33-1 124-20-9, Spermidine 126-07-8 126-72-7 127-00-4, 1-Chloro-2-propanol 128-37-0, BHT, biological studies 129-00-0, Pyrene, biological studies 129-03-3, Cyproheptadine 130-16-5, 5-Chloro-8-hydroxyquinoline 133-06-2, Captan 133-07-3, Folpet 134-32-7, 1-Naphthylamine 134-90-7, L-(+)-threo-Chloramphenicol 137-58-6, Lidocaine 140-79-4, 1,4-Dinitrosopiperazine 145-48-2, 2-Quinizarinsulfonic acid 146-59-8, ICR 170 148-24-3, 8-Hydroxyquinoline, biological studies 148-82-3, Melphalan 149-29-1, Patulin 150-68-5, Monuron **150-70-9** 151-56-4, Ethylenimine, biological studies 151-67-7
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(mutagenicity of, Computer Automated Structure Evaluation for study of structural determinants in relation to)

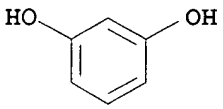
L67 ANSWER 18 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:83178 HCAPLUS
DOCUMENT NUMBER: 112:83178
TITLE: Reportable quantity adjustments; delisting of ammonium thiosulfate
CORPORATE SOURCE: United States Environmental Protection Agency, Washington, DC, 20460, USA
SOURCE: Federal Register (**1989**), 54(155), 33426-84, 14 Aug 1989
CODEN: FEREAC; ISSN: 0097-6326
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Under the Federal Comprehensive Environmental Response, Compensation, and Liability Act, the EPA is promulgating final reportable quantities (RQ) for 258 hazardous substances and hazardous waste streams. NH4 thiosulfate is removed from the list of hazardous substances since the median lethal concn. is well above 500 mg/L for aquatic toxicity. Also included in this final rule is replacement of the registered trademark Gelthane with the generic name difocal, as several companies manuf. this substance.
IT **86-50-0**, Guthion **108-46-3**, 1,3-Benzenediol,

biological studies
RL: POL (Pollutant); OCCU (Occurrence)
(environmental pollution from release of, reportable quantity for, in USA)

RN 86-50-0 HCAPLUS
CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



CC 59-2 (Air Pollution and Industrial Hygiene)
Section cross-reference(s): 60, 61

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RL: POL (Pollutant); OCCU (Occurrence)
(environmental pollution from release of, reportable quantity for, in USA)

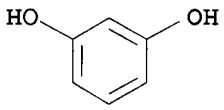
L67 ANSWER 19 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:624600 HCAPLUS
DOCUMENT NUMBER: 111:224600
TITLE: Determination of phenols by azo coupling reaction using 1-(fluoren-2-yl)-3,3-diethyltriazene
AUTHOR(S): Kupletskaya, N. B.; Tikhonova, T. N.; Kashin, A. N.
CORPORATE SOURCE: Moscow State Univ., Moscow, USSR
SOURCE: Zhurnal Analiticheskoi Khimii (**1988**), 43(11), 2070-3

CODEN: ZAKHA8; ISSN: 0044-4502
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB A reflection spectrophotometric method is described for fast quant. and semiquant. detn. of phenols. It is based on an azo coupling reaction and uses 1-(fluoren-2-yl)-3,3-diethyltriazene (I) as a source of diazonium. The reaction is preformed on a chromatog. paper which was satd. with Me2CO soln. of I, dried, and kept in HCl vapor shortly before introduction of a phenol in an alk. aq. soln. Phenols were detd. in concn. range 5 + 10-5-5 + 10-3M. This method was not suitable for detn. of phenols with electron accepting substituents (p-chlorophenol, 2,4-dichlorophenol, nitrophenols) or for hydroquinone and p-aminophenol.

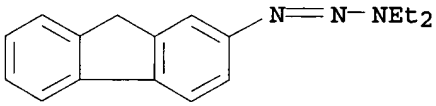
IT **108-46-3**, 1,3-Benzenediol, analysis
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by azo coupling with fluorenyldiethyltriazene and spectrophotometry)

RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



IT **123852-79-9P**
RL: SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)
(prepn. and use of, in detn. of phenols by spectrophotometry)

RN 123852-79-9 HCAPLUS
CN 1-Triazene, 3,3-diethyl-1-(9H-fluoren-2-yl)- (9CI) (CA INDEX NAME)



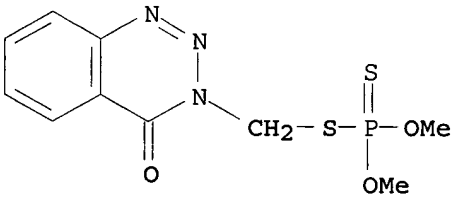
CC 80-6 (Organic Analytical Chemistry)

IT 95-48-7, o-Cresol, analysis 95-55-6, o-Aminophenol 95-65-8, 3,4-Dimethylphenol 106-44-5, analysis 108-43-0, m-Chlorophenol **108-46-3**, 1,3-Benzenediol, analysis 108-95-2, Phenol, analysis 120-80-9, 1,2-Benzenediol, analysis
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by azo coupling with fluorenyldiethyltriazene and spectrophotometry)

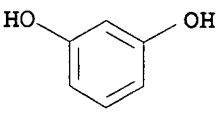
IT **123852-79-9P**
RL: SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)
(prepn. and use of, in detn. of phenols by spectrophotometry)

L67 ANSWER 20 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:491777 HCAPLUS
DOCUMENT NUMBER: 111:91777
TITLE: Use of aquatic lethality tests to estimate safe toxicant concentrations for initial ecological risk assessments

AUTHOR(S): Holcombe, Gary W.; Phipps, Gary L.; Veith, Gilman D.
CORPORATE SOURCE: Environ. Res. Lab., U. S. Environ. Prot. Agency, Duluth, MN, 55804, USA
SOURCE: ASTM Special Technical Publication (**1988**), 1007(Aquat. Toxicol. Environ. Fate: 11th Vol.), 442-58
CODEN: ASTTA8; ISSN: 0066-0558
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB This article presents an approach which allows the body of comparative toxicity data to be used in initial ecol. risk assessments to extrapolate from an acute test with an indicator species to an est. of the no-effect concn. in the environment. The fathead minnow (Pimephales promelas) acute value was selected as the ref. value since this ecotoxicity endpoint has the largest data base for comparative toxicity comparisons. Comparative toxicity endpoints for fish and invertebrates were collected from various sources. When data for all ecotoxicity endpoints are plotted for all chems., this plot can be analyzed statistically using regression anal. to calc. an equation defining the upper 95 percentile prediction limit. The upper 95% prediction limit uses the ref. test (fathead 96-h acute value) to calc. a concn. that would be safe for 95% of the species and chems., assuming that enough comparative toxicol. data (esp. chronic endpoints) are included in the data set.
IT **86-50-0**, Guthion **108-46-3**, Resorcinol, biological studies
RL: BIOL (Biological study)
(no-effect concns. of, in environment, prediction method from aquatic lethality tests in relation to)
RN 86-50-0 HCAPLUS
CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



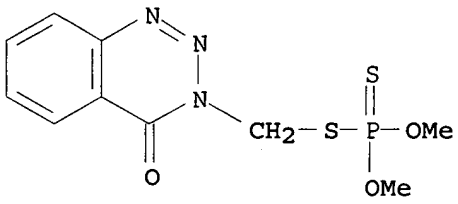
RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



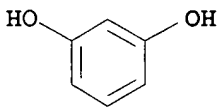
CC 4-1 (Toxicology)
IT 56-23-5, Carbon tetrachloride, biological studies 58-89-9, Lindane 63-25-2, Sevin 67-56-1, Methanol, biological studies 67-72-1, Hexachloroethane 68-12-2, Dimethylformamide, biological studies 72-20-8, Endrin 72-43-5, Methoxychlor 75-09-2, Methylene chloride, biological studies 75-35-4, 1,1-Dichloroethylene,

biological studies 76-01-7, Pentachloroethane 76-44-8, Heptachlor 78-83-1, 2-Methyl-1-propanol, biological studies 79-00-5, 1,1,2-Trichloroethane 79-34-5, 1,1,2,2-Tetrachloroethane 83-32-9, Acenaphthene **86-50-0**, Guthion 87-68-3, Hexachlorobutadiene 87-86-5, Pentachlorophenol 91-20-3, Naphthalene, biological studies 95-48-7, o-Cresol, biological studies 95-49-8, o-Chlorotoluene 99-35-4, 1,3,5-Trinitrobenzene 100-52-7, Benzaldehyde, biological studies 105-75-9, Dibutylfumarate 106-44-5, p-Cresol, biological studies 106-46-7, 1,4-Dichlorobenzene 106-51-4, p-Benzoquinone, biological studies 107-02-8, Acrolein, biological studies 107-06-2, 1,2-Dichloroethane, biological studies 107-07-3, 2-Chloroethanol, biological studies 107-41-5, 2-Methyl-2,4-pentanediol 108-39-4, m-Cresol, biological studies **108-46-3**, Resorcinol, biological studies 108-95-2, Phenol, biological studies 111-90-0, 2-(2-Ethoxy-ethoxy)-ethanol 115-20-8, 2,2,2-Trichloroethanol 115-29-7, Endosulfan 115-32-2, Kelthane 120-80-9, Catechol, biological studies 120-82-1, 1,2,4-Trichlorobenzene 123-31-9, Hydroquinone, biological studies 123-54-6, 2,4-Pentanedione, biological studies 127-18-4, Tetrachloroethylene, biological studies 133-06-2, Captan 139-13-9 298-04-4, Disulfoton 302-01-2, Hydrazine, biological studies 333-41-5, Diazinon 541-73-1, 1,3-Dichlorobenzene 584-79-2 1204-21-3 1582-09-8, Trifluralin 1912-24-9, Atrazine 2921-88-2, Dursban 3698-83-7, 1,3-Dichloro-4,6-dinitrobenzene 8001-35-2, Toxaphene 8065-48-3, Systox 12789-03-6, Chlordane 28434-00-6, s-Bioallethrin 51630-58-1, Pydrin 52645-53-1, Permethrin
RL: BIOL (Biological study)
(no-effect concns. of, in environment, prediction method from aquatic lethality tests in relation to)

L67 ANSWER 21 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:218230 HCAPLUS
DOCUMENT NUMBER: 110:218230
TITLE: Air contaminants
CORPORATE SOURCE: United States Occupational Safety and Health Administration, Washington, DC, 20210, USA
SOURCE: Federal Register (**1989**), 54(12, Bk. 2), 2332-983, 19 Jan 1989
CODEN: FEREAC; ISSN: 0097-6326
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Under the Federal Occupational Safety and Health act, OSHA is amending existing air containment stds. and setting new permissible exposure limits for toxic substances commonly used in the workplace.
IT **86-50-0**, Azinphos-methyl **108-46-3**, Resorcinol, biological studies
RL: ADV (Adverse effect, including toxicity); POL (Pollutant); BIOL (Biological study); OCCU (Occurrence)
(air pollution by, occupational exposure to, stds. for, in USA)
RN 86-50-0 HCAPLUS
CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



CC 59-5 (Air Pollution and Industrial Hygiene)
Section cross-reference(s): 4
IT 50-00-0, Formaldehyde, biological studies 50-29-3, biological studies 50-32-8, Benzo[a]pyrene, biological studies 50-78-2 53-96-3 54-11-5, Nicotine 55-38-9, Fenthion 55-63-0, Nitroglycerin 56-23-5, biological studies 56-38-2, Parathion 56-81-5, 1,2,3-Propanetriol, biological studies 57-14-7, 1,1-Dimethylhydrazine 57-24-9, Strychnine 57-50-1, biological studies 57-57-8, 2-Oxetanone 58-89-9, Lindane 60-11-7, 4-Dimethylaminoazobenzene 60-29-7, Ethyl ether, biological studies 60-34-4, Methyl hydrazine 60-57-1, Dieldrin 61-82-5, Amitrole 62-53-3, Aniline, biological studies 62-73-7, Dichlorvos 62-74-8, Sodium fluoroacetate 62-75-9, N-Nitrosodimethylamine 63-25-2 64-17-5, Ethyl alcohol, biological studies 64-18-6, Formic acid, biological studies 64-19-7, Acetic acid, biological studies 67-56-1, Methyl alcohol, biological studies 67-63-0, Isopropyl alcohol, biological studies 67-64-1, Acetone, biological studies 67-66-3, Chloroform, biological studies 67-72-1, Hexachloroethane 68-11-1, Thioglycolic acid, biological studies 68-12-2, Dimethylformamide, biological studies 71-23-8, n-Propyl alcohol, biological studies 71-36-3, n-Butyl alcohol, biological studies 71-43-2, Benzene, biological studies 71-55-6, Methyl chloroform 72-20-8, Endrin 72-43-5, Methoxychlor 74-83-9, Methyl bromide, biological studies 74-87-3, Methyl chloride, biological studies 74-88-4, biological studies 74-89-5, Methylamine, biological studies 74-90-8, Hydrogen cyanide, biological studies 74-93-1, Methyl mercaptan, biological studies 74-96-4, Ethyl bromide 74-97-5, Chlorobromomethane 74-98-6, Propane, biological studies 74-99-7, Methyl acetylene 75-00-3, Ethyl chloride 75-01-4, biological studies 75-04-7, Ethylamine, biological studies 75-05-8, Acetonitrile, biological studies 75-07-0, Acetaldehyde, biological studies 75-08-1, Ethyl mercaptan 75-09-2, Methylene chloride, biological studies 75-12-7, Formamide, biological studies 75-15-0, Carbon disulfide, biological studies 75-21-8, Oxirane, biological studies 75-25-2, Bromoform 75-31-0, Isopropylamine, biological studies 75-34-3, 1,1-Dichloroethane 75-35-4, Vinylidene chloride, biological studies 75-43-4, Dichloromonofluoromethane 75-44-5, Phosgene 75-45-6, Chlorodifluoromethane 75-47-8, Iodoform 75-50-3, Trimethylamine, biological studies 75-52-5, Nitromethane,

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75-65-0, tert-Butyl alcohol, biological studies 75-69-4,
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Tetramethyl lead 75-99-0, 2,2-Dichloropropionic acid 76-03-9,
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1,1,2,2-Tetrachloro-1,2-difluoroethane 76-13-1,
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79-00-5, 1,1,2-Trichloroethane 79-01-6, biological studies
79-04-9, Chloroacetyl chloride 79-06-1, 2-Propenamide, biological
studies 79-09-4, Propionic acid, biological studies 79-10-7,
2-Propenoic acid, biological studies 79-20-9, Methyl acetate
79-24-3, Nitroethane 79-27-6, Acetylene tetrabromide 79-34-5,
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phthalate 85-00-7 85-44-9, Phthalic anhydride **86-50-0**,
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92-87-5, Benzidine 92-93-3, 4-Nitrodiphenyl 93-76-5 94-36-0,
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phenol, biological studies 95-49-8, o-Chlorotoluene 95-50-1,
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Trichloropropane 96-22-0, Diethyl ketone 96-33-3 96-69-5,
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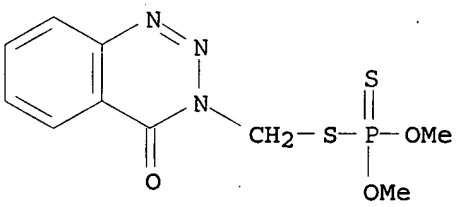
98-95-3, Nitrobenzene, biological studies 99-08-1, m-Nitrotoluene
99-65-0, 1,3-Dinitrobenzene 99-99-0, p-Nitrotoluene 100-00-5,
p-Nitrochlorobenzene 100-01-6, biological studies 100-25-4
100-37-8 100-41-4, Ethyl benzene, biological studies 100-42-5,
biological studies 100-44-7, Benzyl chloride, biological studies
100-61-8, biological studies 100-63-0 100-74-3,
N-Ethylmorpholine 101-14-4, 4,4'-Methylene bis(2-chloroaniline)
101-68-8 101-84-8, Phenyl ether 102-54-5, Dicyclopentadienyl
iron 102-81-8 104-94-9, p-Anisidine 105-46-4, sec-Butyl
acetate 105-60-2, biological studies 106-35-4, 3-Heptanone
106-42-3, p-Xylene, biological studies 106-44-5, 4-Methylphenol,
biological studies 106-46-7, p-Dichlorobenzene 106-49-0,
p-Toluidine, biological studies 106-50-3, p-Phenylene diamine,
biological studies 106-51-4, 2,5-Cyclohexadiene-1,4-dione,
biological studies 106-68-3, Ethyl amyl ketone 106-87-6
106-89-8, Epichlorohydrin, biological studies 106-92-3, Allyl
glycidyl ether 106-93-4, Ethylene dibromide 106-97-8, Butane,
biological studies 106-99-0, 1,3-Butadiene, biological studies
107-02-8, Acrolein, biological studies 107-05-1, Allyl chloride
107-06-2, Ethylene dichloride, biological studies 107-07-3,

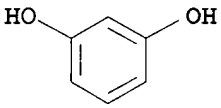
Ethylene chlorohydrin, biological studies 107-13-1, Acrylonitrile, biological studies 107-15-3, 1,2-Ethanediamine, biological studies 107-18-6, Allyl alcohol, biological studies 107-19-7, Propargyl alcohol 107-20-0, Chloroacetaldehyde 107-21-1, 1,2-Ethanediol, biological studies 107-30-2, Chloromethyl methyl ether 107-31-3, Methyl formate 107-41-5, Hexylene glycol 107-49-3, TEPP 107-66-4, Dibutyl phosphate 107-87-9, 2-Pentanone 108-03-2, 1-Nitropropane 108-05-4, Vinyl acetate, biological studies 108-10-1, Hexone 108-11-2, Methyl isobutyl carbinol 108-18-9, Diisopropylamine 108-20-3, Isopropyl ether 108-21-4, Isopropyl acetate 108-24-7, Acetic anhydride 108-31-6, 2,5-Furandione, biological studies 108-38-3, m-Xylene, biological studies 108-39-4, 3-Methylphenol, biological studies 108-44-1, m-Toluidine, biological studies **108-46-3**, Resorcinol, biological studies 108-83-8, Diisobutyl ketone 108-84-9 108-87-2, Methylcyclohexane 108-88-3, biological studies 108-90-7, Chlorobenzene, biological studies 108-91-8, Cyclohexanamine, biological studies 108-93-0, Cyclohexanol, biological studies 108-94-1, Cyclohexanone, biological studies 108-95-2, Phenol, biological studies 108-98-5, Phenyl mercaptan, biological studies 109-59-1, 2-Isopropoxyethanol 109-60-4, n-Propyl acetate 109-66-0, Pentane, biological studies 109-73-9, Butylamine, biological studies 109-79-5, Butyl mercaptan 109-86-4, Methyl cellosolve
RL: ADV (Adverse effect, including toxicity); POL (Pollutant); BIOL (Biological study); OCCU (Occurrence)
(air pollution by, occupational exposure to, stds. for, in USA)

L67 ANSWER 22 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:569090 HCAPLUS
DOCUMENT NUMBER: 103:169090
TITLE: A concise feature set for the pattern recognition of low-temperature luminescence spectra of hazardous chemicals
AUTHOR(S): Sogliero, Gene; Eastwood, DeLyle; Gilbert, James
CORPORATE SOURCE: Dep. Clin. Res., Pfizer Cent. Res., Groton, CT, 06340, USA
SOURCE: ASTM Special Technical Publication (**1985**), 863(Adv. Lumin. Spectrosc.), 95-115
CODEN: ASTTA8; ISSN: 0066-0558
DOCUMENT TYPE: Journal
LANGUAGE: English
AB As computer libraries of cor., digitized, low-temp. luminescence, and fluorescence spectra are expanded, it becomes increasingly important to specify a succinct and pithy set of features that will accelerate the library search for a matched spectrum ot an unknown sample spectrum. While feature sets for other types of spectra have been investigated extensively, feature sets for fluorescence and luminescence spectra have not been fully explored as yet. Using a specially generated library of low-temp. luminescence spectra of ≈60 hazardous chems., a feature set consisting of only 6 components (the 1st 4 noncentral sample moments of the spectrum, the approx. normalized area under the spectral envelope, and the wavelength corresponding to the location of the max. intensity) performs exceptionally well in a test using a cluster anal. involving >2000 pairwise comparisons of the feature sets.
IT **86-50-0 108-46-3**, properties
RL: PRP (Properties)
(luminescence of, pattern recognition of low-temp.)
RN 86-50-0 HCAPLUS

CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



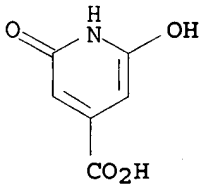
CC 73-5 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 79, 80
IT 56-72-4 63-25-2 65-85-0, properties 69-72-7, properties 71-43-2, properties 72-43-5 72-54-8 80-05-7, properties 83-32-9 84-66-2 84-74-2 85-68-7 **86-50-0** 87-66-1 87-86-5 88-06-2 88-99-3, properties 90-13-1 91-20-3, properties 91-22-5, properties 94-75-7, properties 95-48-7, properties 98-01-1, properties 100-41-4, properties 100-42-5, properties 100-46-9, properties 100-51-6, properties 101-84-8 104-15-4, properties 106-43-4 106-46-7 106-48-9 106-49-0, properties **108-46-3**, properties 108-68-9 110-62-3 119-61-9, properties 120-12-7, properties 120-80-9, properties 120-83-2 121-91-5, properties 122-39-4, properties 123-31-9, properties 129-00-0, properties 206-44-0 260-94-6 275-51-4 330-54-1 1194-65-6 1330-78-5 1918-00-9 2921-88-2 7782-41-4, properties 10102-06-4 25154-52-3
RL: PRP (Properties)
(luminescence of, pattern recognition of low-temp.)

L67 ANSWER 23 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:401655 HCAPLUS
DOCUMENT NUMBER: 103:1655
TITLE: Acute oral toxicity and repellency of 933 chemicals to house and deer mice
AUTHOR(S): Schafer, E. W., Jr.; Bowles, W. A., Jr.
CORPORATE SOURCE: Denver Wildl. Res. Cent., Fish Wildl. Serv., Denver, CO, 80225, USA
SOURCE: Archives of Environmental Contamination and Toxicology (**1985**), 14(1), 111-29
CODEN: AECTCV; ISSN: 0090-4341
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Five individual bioassay repellency or toxicity variables were estd. or detd. for deer mice (Peromyscus maniculatus) and house mice (Mus musculus) under lab. conditions. ALD's (Approx. LDs) or LD50's of 230 chems. to deer mice are presented, as are food redn. (FR) values

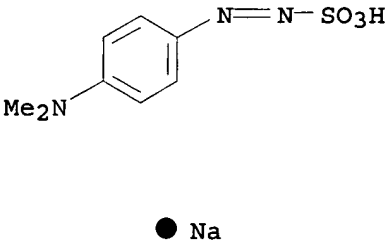
(3-day feeding test as a 2.0% treatment rate) for white wheat seeds (Triticum aestivum) for 696 chems. and for Douglas fir seeds (Pseudotsuga menziesii) for 81 chems. A similar repellency evaluation (REP) using a 5-day test with white wheat seeds at a 2.0% treatment rate was conducted with house mice and the results for 347 chems. are presented. These toxicity and repellency data should be useful to those desiring to predict the potential for acute toxicity in wild mammals following exposure to a wide variety of chems. A calcn. of the daily chem. dose ingested in mg/kg/day during the wheat test on deer mice and its resultant effects on mortality are also presented for most of the 696 chems. This calcd. value, when used along with the ALD or LD50, should permit a rough est. of the potential subacute toxicity of any tested chem. on wild mammals for which both types of data are available.

IT **99-11-6 140-56-7 1933-50-2**
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(toxicity of, to deer mouse and house mouse, repellency in relation to)

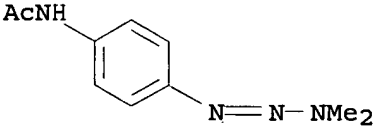
RN 99-11-6 HCAPLUS
CN 4-Pyridinecarboxylic acid, 1,2-dihydro-6-hydroxy-2-oxo- (9CI) (CA INDEX NAME)



RN 140-56-7 HCAPLUS
CN Diazenesulfonic acid, [4-(dimethylamino)phenyl]-, sodium salt (9CI) (CA INDEX NAME)



RN 1933-50-2 HCAPLUS
CN Acetamide, N-[4-(3,3-dimethyl-1-triazenyl)phenyl]- (9CI) (CA INDEX NAME)



CC 4-3 (Toxicology)
IT 50-65-7 50-71-5 51-73-0 51-79-6 52-60-8 52-66-4 54-96-6
55-37-8 55-38-9 56-35-9 56-36-0 56-53-1 56-72-4 57-24-9
57-47-6 58-36-6 59-31-4 59-49-4 60-23-1 60-51-5 60-54-8
61-28-9 62-23-7 63-25-2 63-75-2 63-98-9 63-99-0 64-10-8
65-49-6 65-85-0, biological studies 66-40-0 66-81-9 67-51-6
70-55-3 72-00-4 72-20-8 72-33-3 74-31-7 74-39-5 75-08-1
75-33-2 75-66-1 76-24-4 76-63-1 76-87-9 77-58-7 77-71-4
77-80-5 78-04-6 78-57-9 79-19-6 79-41-4, biological studies
80-08-0 80-12-6 80-22-8 80-59-1 81-15-2 81-81-2 82-43-9
82-45-1 83-01-2 83-07-8 83-34-1 84-66-2 85-02-9 85-59-6
85-98-3 86-53-3 87-47-8 87-51-4, biological studies 87-66-1
87-88-7 88-04-0 88-12-0, biological studies 88-14-2 88-29-9
89-00-9 89-02-1 89-25-8 89-35-0 89-62-3 89-69-0 90-01-7
91-02-1 91-63-4 92-13-7 92-52-4, biological studies 92-53-5
92-59-1 92-70-6 92-82-0 92-84-2 93-04-9 93-10-7 93-18-5
93-46-9 93-75-4 94-09-7 94-18-8 94-52-0 94-86-0 95-03-4
95-64-7 95-69-2 95-71-6 95-76-1 95-79-4 95-86-3 95-88-5
96-12-8 96-24-2 96-31-1 96-45-7 96-48-0 96-50-4 96-53-7
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98-58-8 98-60-2 99-09-2 **99-11-6** 99-55-8 99-59-2
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biological studies 100-26-5 100-35-6 100-48-1 100-52-7,
biological studies 100-54-9 100-55-0 100-70-9 100-71-0
100-97-0, biological studies 101-05-3 101-59-7 101-75-7
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120-93-4 121-60-8 121-66-4 121-71-1 121-75-5 122-14-5
122-15-6 122-66-7 122-88-3 123-69-3 123-75-1, biological
studies 124-12-9 126-14-7
RL: ADV (Adverse effect, including toxicity); BIOL (Biological
study)
(toxicity of, to deer mouse and house mouse, repellency in
relation to)
IT 127-07-1 130-15-4 130-95-0 131-09-9 131-22-6 132-75-2
133-06-2 133-07-3 134-19-0 134-20-3 135-88-6 136-77-6
136-95-8 137-06-4 137-07-5 137-26-8 137-30-4 139-65-1
140-53-4 **140-56-7** 141-66-2 141-86-6 142-08-5
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RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(toxicity of, to deer mouse and house mouse, repellency in relation to)

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5978-34-7 6046-93-1 6164-98-3
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(toxicity of, to deer mouse and house mouse, repellency in relation to)

L67 ANSWER 24 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:130001 HCAPLUS
DOCUMENT NUMBER: 100:130001
TITLE: Heat-sensitive and photofixing recording sheet with diazosulfonate and its acidic coupling agent
INVENTOR(S): Takiguchi, Ryohei; Nagashima, Masayoshi
PATENT ASSIGNEE(S): Dai Nippon Printing Co., Ltd., Japan; Toshiba Corp.
SOURCE: U.S., 9 pp. Cont.-in-part of U.S. Ser. No. 174,443, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4421839	A	19831220	US 1982-354525	19820303
JP 56053090	A2	19810512	JP 1979-128816 <--	19791008
JP 01007879	B4	19890210		
JP 56053091	A2	19810512	JP 1979-128817	19791008

PRIORITY APPLN. INFO.:

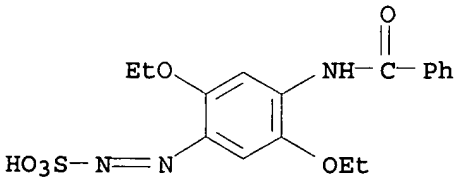
JP 1979-U107358	A	197908 03
JP 1979-U107359	A	197908 03
JP 1979-U107360	A	197908 03
JP 1979-U107361	A	197908 03
JP 1979-128816	A	197910 08
JP 1979-128817	A	197910 08
US 1980-174443	A2	198008 01

AB A thermal recording heat-sensitive layer contains a diazosulfonate, an acidic coupling agent, and a member selected from a group consisting of thermosetting or thermoplastic resins having a glass transition point of 70-150°. Thus, a coated paper support was coated with a compn. contg. Na 4-(4'-tolylmercapto)-2,5-diethoxybenzenesulfonate 3, Me cellosolve 9, 2-hydroxy-3-naphthoic acid 2, Sumipex B-MHO 5, MeCOEt 67 g, dried at 60° for 1 min, activated by flood exposure with a Xe lamp, and used for recording with a dot-type thermal head (15 V, 50 ms) to give clear blue images, which were fixed with diazo copying chem. lamp illumination.

IT **36429-18-2 36429-19-3 48193-85-7**
RL: USES (Uses)
(thermal recording compn. contg. acidic coupling agent and, photofixing of images in)

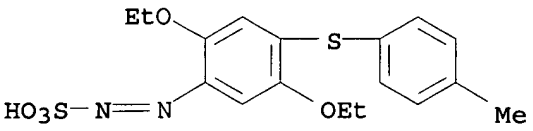
RN 36429-18-2 HCAPLUS

CN Diazenesulfonic acid, [4-(benzoylamino)-2,5-diethoxyphenyl]-, monosodium salt (9CI) (CA INDEX NAME)

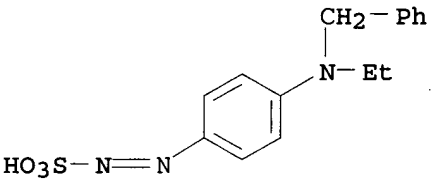


● Na

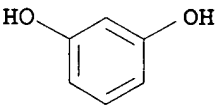
RN 36429-19-3 HCAPLUS
CN Diazenesulfonic acid, [2,5-diethoxy-4-[(4-methylphenyl)thio]phenyl]-, sodium salt (9CI) (CA INDEX NAME)



RN 48193-85-7 HCAPLUS
CN Diazenesulfonic acid, [4-[ethyl(phenylmethyl)amino]phenyl]- (9CI) (CA INDEX NAME)



IT **108-46-3**, uses and miscellaneous
RL: USES (Uses)
(thermal recording compn. contg. diazosulfonate and, photofixing of images in)
RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



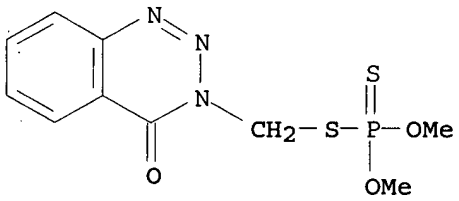
IC G03C001-56; G03C001-58
INCL 430164000
CC 74-12 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
IT **36429-18-2 36429-19-3 48193-85-7**
RL: USES (Uses)
(thermal recording compn. contg. acidic coupling agent and, photofixing of images in)
IT 69-72-7, uses and miscellaneous 92-70-6 99-50-3 102-01-2
108-46-3, uses and miscellaneous 2283-08-1 16534-12-6
89308-02-1
RL: USES (Uses)
(thermal recording compn. contg. diazosulfonate and, photofixing of images in)

L67 ANSWER 25 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1983:465537 HCAPLUS
DOCUMENT NUMBER: 99:65537
TITLE: The acute oral toxicity, repellency, and hazard potential of 998 chemicals to one or more species of wild and domestic birds
AUTHOR(S): Schafer, E. W., Jr.; Bowles, W. A., Jr.; Hurlbut, J.
CORPORATE SOURCE: Wildl. Res. Cent., U. S. Fish Wildl. Serv., Denver, CO, 80225, USA
SOURCE: Archives of Environmental Contamination and Toxicology (1983), 12(3), 355-82
CODEN: AECTCV; ISSN: 0090-4341
DOCUMENT TYPE: Journal
LANGUAGE: English

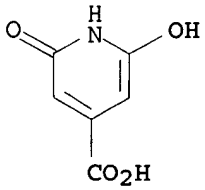
AB The acute oral toxicity, repellency, and hazard potential of 998 chem. to 1 or more of 68 species of wild and domestic birds was detd. by standardized testing procedures. Red-winged blackbirds (Agelaius phoeniceus) were the most sensitive of the bird species tested on a large no. of chems., and an index based on red-wing toxicity and repellency may provide an appropriate indication of the probability of acute avian poisoning episodes. Avian repellency and toxicity were not pos. correlated (i.e., toxicity varied independently with repellency).

IT **86-50-0 99-11-6 140-56-7**
591-27-5 1933-50-2
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(toxicity of, to birds, repellency in relation to)

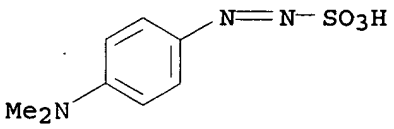
RN 86-50-0 HCAPLUS
CN Phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (6CI, 9CI) (CA INDEX NAME)



RN 99-11-6 HCAPLUS
CN 4-Pyridinecarboxylic acid, 1,2-dihydro-6-hydroxy-2-oxo- (9CI) (CA INDEX NAME)

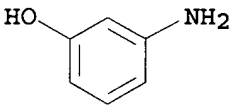


RN 140-56-7 HCAPLUS
CN Diazenesulfonic acid, [4-(dimethylamino)phenyl]-, sodium salt (9CI) (CA INDEX NAME)

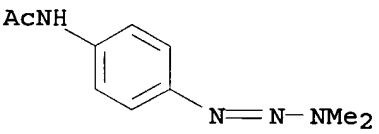


● Na

RN 591-27-5 HCAPLUS
CN Phenol, 3-amino- (9CI) (CA INDEX NAME)



RN 1933-50-2 HCAPLUS
CN Acetamide, N-[4-(3,3-dimethyl-1-triazenyl)phenyl]- (9CI) (CA INDEX NAME)



CC 4-4 (Toxicology)
Section cross-reference(s): 1, 5
IT 50-06-6, biological studies 50-07-7 50-09-9 50-11-3 50-37-3
50-53-3, biological studies 50-55-5 50-65-7 50-71-5 50-76-0
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biological studies 95-55-6 95-57-8 95-64-7 95-69-2 95-71-6
95-74-9 95-76-1 95-79-4 96-24-2 96-27-5 96-48-0 96-50-4
96-96-8 96-99-1 97-17-6 97-18-7 97-50-7
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(toxicity of, to birds, repellency in relation to)

IT 97-53-0 97-54-1 97-77-8 98-01-1, biological studies 98-03-3
98-07-7 98-11-3, biological studies 98-29-3 98-82-8 98-98-6
99-05-8 99-09-2 **99-11-6** 99-30-9 99-43-4 99-55-8
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100-22-1 100-35-6 100-43-6 100-47-0, biological studies
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299-85-4 299-86-5 300-62-9
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(toxicity of, to birds, repellency in relation to)

IT 302-17-0 303-01-5 304-91-6 309-00-2 309-43-3 313-05-3
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1688-71-7 1746-01-6 1754-58-1 1757-18-2 1758-68-5
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(toxicity of, to birds, repellency in relation to)

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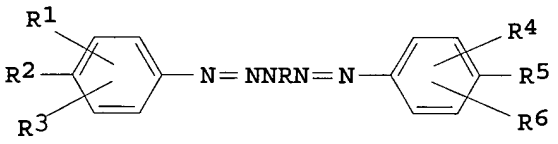
15590-77-9
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(toxicity of, to birds, repellency in relation to)

L67 ANSWER 26 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1978:113351 HCAPLUS

DOCUMENT NUMBER: 88:113351
TITLE: Diazo copying sheet for negative copies
INVENTOR(S): Chmatal, Vladimir; Remes, Miroslav; Zverina, Vladimir; Matrka, Miroslav; Kroupa, Jaroslav; Gorgon, Oldrich
PATENT ASSIGNEE(S): Czech.
SOURCE: Czech., 4 pp.
CODEN: CZXXA9
DOCUMENT TYPE: Patent
LANGUAGE: Czech
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CS 169589	B	19760729	CS 1974-7427 <--	197410 31
PRIORITY APPLN. INFO.:			CS 1974-7427 A <--	197410 31

GI

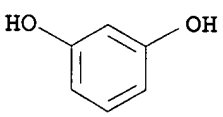


I

AB A pentaazadiene deriv. I (R = C1-4 alkyl, R1-R6 = H, Me, OMe, OEt, NEt2, morpholino) is combined with a coupling compd., a sensitizer, a stabilizer, and other additives to give a photosensitive compn. for manuf. of a diazo sheet for neg. copies. Thus, a triacetate film support was coated with an emulsion contg. 1,5-diphenyl-3-methyl-1,4-pentaazadiene 1.5, 2-hydroxy-3-naphthoic acid 2-methoxyanilide 1.3, morpholine 1, thiourea 0.5, cellulose acetate 2.5 g, MeOCH2CH2OH 40, and Me2CO 40 mL. After exposure and stabilization, the copying film gave a brilliant red image with clear background.

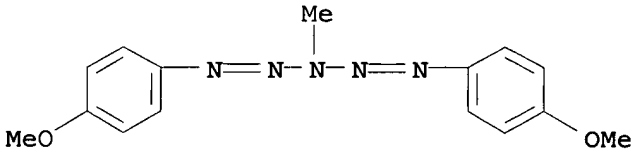
IT **108-46-3**, uses and miscellaneous
RL: USES (Uses)
(photosensitive compns. contg. pentaazadiene deriv. and, for diazo copying materials for neg. copy prodn.)

RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)

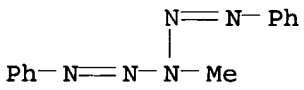


IT **41798-80-5 41798-82-7 65882-01-1**
65882-02-2 65882-03-3 65882-04-4
RL: USES (Uses)
(photosensitive compns. contg., for diazo copying materials for neg. copy prodn.)

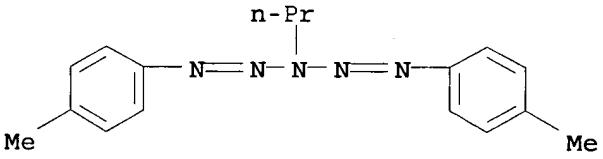
RN 41798-80-5 HCAPLUS
CN 1,4-Pentazadiene, 1,5-bis(4-methoxyphenyl)-3-methyl- (9CI) (CA INDEX NAME)



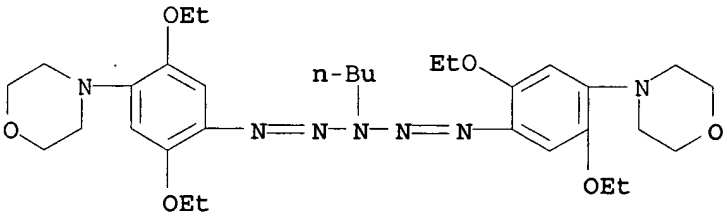
RN 41798-82-7 HCAPLUS
CN 1,4-Pentazadiene, 3-methyl-1,5-diphenyl- (6CI, 9CI) (CA INDEX NAME)



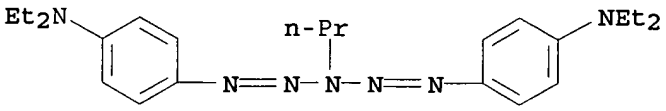
RN 65882-01-1 HCAPLUS
CN 1,4-Pentazadiene, 1,5-bis(4-methylphenyl)-3-propyl- (9CI) (CA INDEX NAME)



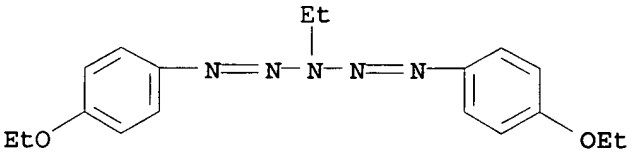
RN 65882-02-2 HCAPLUS
CN Morpholine, 4,4'-[(3-butyl-1,4-pentazadiene-1,5-diyl)bis(2,5-diethoxy-4,1-phenylene)]bis- (9CI) (CA INDEX NAME)



RN 65882-03-3 HCAPLUS
CN Benzenamine, 4,4'-(3-propyl-1,4-pentazadiene-1,5-diyl)bis[N,N-diethyl- (9CI) (CA INDEX NAME)



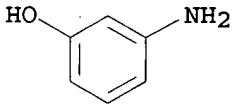
RN 65882-04-4 HCAPLUS
CN 1,4-Pentazadiene, 1,5-bis(4-ethoxyphenyl)-3-ethyl- (9CI) (CA INDEX NAME)



IC G03C005-18
CC 74-3 (Radiation Chemistry, Photochemistry, and Photographic Processes)
IT **108-46-3**, uses and miscellaneous 108-73-6 131-55-5 135-62-6 10155-47-2 27438-39-7
RL: USES (Uses)
(photosensitive compns. contg. pentaazadiene deriv. and, for diazo copying materials for neg. copy prodn.)
IT **41798-80-5 41798-82-7 65882-01-1 65882-02-2 65882-03-3 65882-04-4**
RL: USES (Uses)
(photosensitive compns. contg., for diazo copying materials for neg. copy prodn.)

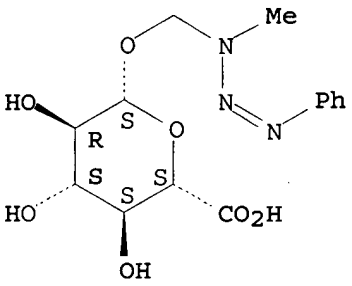
L67 ANSWER 27 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1977:546779 HCAPLUS
DOCUMENT NUMBER: 87:146779
TITLE: Metabolism and bioactivation of 3,3-dimethyl-1-phenyltriazene and its 4-chlorophenyl analog
AUTHOR(S): Kolar, G. F.
CORPORATE SOURCE: Inst. Toxicol. Chemother., German Cancer Res. Cent., Heidelberg, Fed. Rep. Ger.
SOURCE: Xenobiotica (**1977**), 7(1-2), 100-1
CODEN: XENOBH; ISSN: 0049-8254
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The major urinary metabolites of 3,3-dimethyl-1-phenyltriazene (I) [**7227-91-0**] in rats were conjugates of aniline (1-2%), and 2-hydroxyaniline (5-7%), 3-hydroxyaniline (.apprx.1%), and 4-hydroxyaniline (31-6%). Metabolites contg. the intact triazene structure (0.9-1.1%) were converted into 4-benzeneazo-N-ethyl-1-naphthylamine [60375-32-8] (0.6-0.7%), 4-(2-hydroxybenzeneazo)-N-ethyl-1-naphthylamine [60375-33-9] (0.02%) and 4-(4-hydroxybenzeazo)-N-ethyl-1-naphthylamine [60375-34-0] (0.3-0.4%). Two labeled triazene metabolites of I were tentatively identified as 3-hydroxymethyl-3-methyl-1-phenyltriazene O-glucuronide [**62782-59-6**] and 1-(4-hydroxyphenyl)-3,3-dimethyltriazene O-glucuronide [**62782-60-9**]. Urinary metabolites of 1-(4-chlorophenyl)-3,3-dimethyltriazene [**7203-90-9**] showed a similar pattern to those of I, but hydroxylation of the ortho position was .apprx.15%, and the yield of 4-chloroaniline was 5%.

IT **591-27-5 62782-59-6 62782-60-9**
RL: BIOL (Biological study)
(dimethylphenyltriazene metabolite, in urine)
RN 591-27-5 HCAPLUS
CN Phenol, 3-amino- (9CI) (CA INDEX NAME)



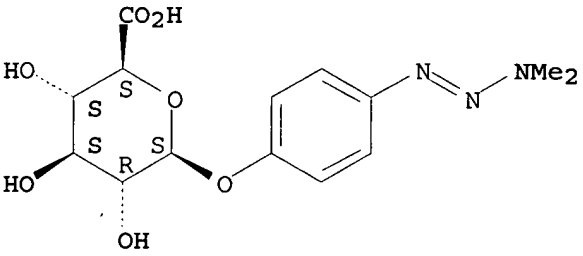
RN 62782-59-6 HCAPLUS
CN β-D-Glucopyranosiduronic acid, (1-methyl-3-phenyl-2-triazenyl)methyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

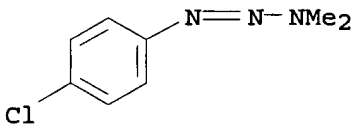


RN 62782-60-9 HCAPLUS
CN β-D-Glucopyranosiduronic acid, 4-(3,3-dimethyl-1-triazenyl)phenyl (9CI) (CA INDEX NAME)

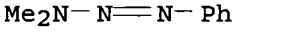
Absolute stereochemistry.
Double bond geometry unknown.



IT **7203-90-9 7227-91-0**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(metab. of)
RN 7203-90-9 HCAPLUS
CN 1-Triazene, 1-(4-chlorophenyl)-3,3-dimethyl- (9CI) (CA INDEX NAME)



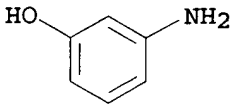
RN 7227-91-0 HCAPLUS
CN 1-Triazene, 3,3-dimethyl-1-phenyl- (9CI) (CA INDEX NAME)



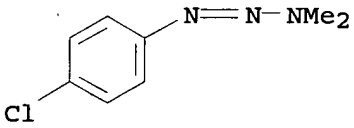
CC 4-7 (Toxicology)
IT 62-53-3, biological studies 95-55-6 123-30-8 **591-27-5**
60375-32-8 60375-33-9 60375-34-0 **62782-59-6**
62782-60-9
RL: BIOL (Biological study)
(dimethylphenyltriazene metabolite, in urine)
IT **7203-90-9 7227-91-0**
RL: BPR (Biological process); BSU (Biological study, unclassified);
BIOL (Biological study); PROC (Process)
(metab. of)

L67 ANSWER 28 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1977:182906 HCAPLUS
DOCUMENT NUMBER: 86:182906
TITLE: Metabolism of the tumor-inhibitory 3,3-dimethyl-1-phenyltriazene and its 4-chlorophenyl analog
AUTHOR(S): Kolar, G. F.; Schlesiger, J.
CORPORATE SOURCE: Ger. Cancer Res. Cent., Inst. Toxicol. Chemother., Heidelberg, Fed. Rep. Ger.
SOURCE: Chemother., Proc. Int. Congr. Chemother., 9th (**1976**), Meeting Date 1975, Volume 8, 91-6. Editor(s): Hellmann, Kurt; Connors, T. A. Plenum: New York, N. Y.
CODEN: 35DFA6
DOCUMENT TYPE: Conference
LANGUAGE: English
AB The s.c. injection of 3,3-dimethyl-1-phenyltriazene [**7227-91-0**] or its para chlorinated congener, 1-(4-chlorophenyl)-3,3-dimethyltriazene [**7203-90-9**] into rats resulted in the excretion of 0.9-1.4% of metabolites capable of diazo coupling after cold acid treatment and of 30-46% of modified anilines. Since the principal azo derivs. were not hydroxylated on the Ph ring, the lipophilic triazenes had to be rendered water-sol. by hydroxylation and subsequent conjugation on the Me group(s) at N-3. The hydroxylating enzymes interacted with the para position of the Ph ring, but when the para position was substituted with Cl, hydroxylation occurred predominantly at the ortho positions. Catabolic degrdn. of 1-(4-chlorophenyl)-3,3-dimethyltriazene, accompanied by an hydroxylation-induced migration of a substituent, was detected for the first time in a cytostatic compd.
IT **591-27-5**
RL: BIOL (Biological study)
(as dimethylphenyltriazene metabolite)
RN 591-27-5 HCAPLUS

CN Phenol, 3-amino- (9CI) (CA INDEX NAME)



IT **7203-90-9 7227-91-0**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(metab. of)
RN 7203-90-9 HCAPLUS
CN 1-Triazene, 1-(4-chlorophenyl)-3,3-dimethyl- (9CI) (CA INDEX NAME)



RN 7227-91-0 HCAPLUS
CN 1-Triazene, 3,3-dimethyl-1-phenyl- (9CI) (CA INDEX NAME)

$Me_2N-N=N-Ph$

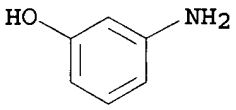
CC 1-2 (Pharmacodynamics)
IT 62-53-3, biological studies 95-55-6 123-30-8 **591-27-5**
60375-32-8 60375-33-9 60375-34-0
RL: BIOL (Biological study)
(as dimethylphenyltriazene metabolite)
IT **7203-90-9 7227-91-0**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(metab. of)

L67 ANSWER 29 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1973:42929 HCAPLUS
DOCUMENT NUMBER: 78:42929
TITLE: Synthesis of biologically active triazenes from isolable diazonium salts
AUTHOR(S): Kolar, G. F.
CORPORATE SOURCE: Chem. Lab., Max-Planck-Inst. Immunbiol., Freiburg/Br., Fed. Rep. Ger.
SOURCE: Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie, Biochemie, Biophysik, Biologie (**1972**), 27(10), 1183-5
CODEN: ZENBAX; ISSN: 0044-3174
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Title compds. RC6H4N:NNMe2 (R = H, o-, m-, p-HO, i-, m-, p-HO2C, o-, m-, p-HO3S) were prepd. by diazotization of RC6H4NH2 in HBF4 or HPF6 giving RC6H4N2+BF4- or RC6H4N2+PF6-, resp., which were treated with Me2NH in aq. soln. in the absence of mineral

base.

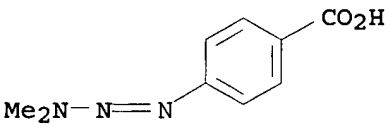
IT **591-27-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(diazotization of, in tetrafluoroboric acid and hexafluorophosphoric acid)

RN 591-27-5 HCAPLUS
CN Phenol, 3-amino- (9CI) (CA INDEX NAME)



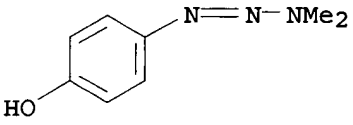
IT **7203-91-0P 7227-91-0P 7227-93-2P**
20119-28-2P 20241-07-0P 35433-91-1P
37599-71-6P 39201-85-9P 39201-86-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 7203-91-0 HCAPLUS
CN Benzoic acid, 4-(3,3-dimethyl-1-triazenyl)- (9CI) (CA INDEX NAME)

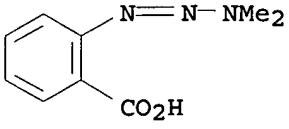


RN 7227-91-0 HCAPLUS
CN 1-Triazene, 3,3-dimethyl-1-phenyl- (9CI) (CA INDEX NAME)

RN 7227-93-2 HCAPLUS
CN Phenol, 4-(3,3-dimethyl-1-triazenyl)- (9CI) (CA INDEX NAME)

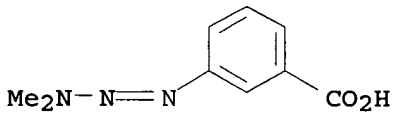


RN 20119-28-2 HCAPLUS
CN Benzoic acid, 2-(3,3-dimethyl-1-triazenyl)- (9CI) (CA INDEX NAME)

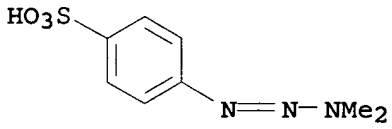


RN 20241-07-0 HCAPLUS

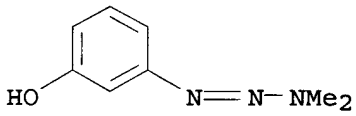
CN Benzoic acid, 3-(3,3-dimethyl-1-triazenyl)- (9CI) (CA INDEX NAME)



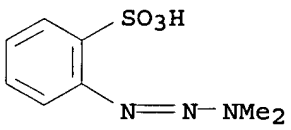
RN 35433-91-1 HCAPLUS
CN Benzenesulfonic acid, 4-(3,3-dimethyl-1-triazenyl)- (9CI) (CA INDEX NAME)



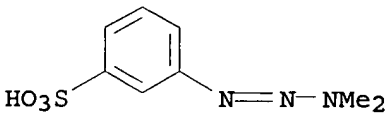
RN 37599-71-6 HCAPLUS
CN Phenol, 3-(3,3-dimethyl-1-triazenyl)- (9CI) (CA INDEX NAME)



RN 39201-85-9 HCAPLUS
CN Benzenesulfonic acid, 2-(3,3-dimethyl-1-triazenyl)- (9CI) (CA INDEX NAME)



RN 39201-86-0 HCAPLUS
CN Benzenesulfonic acid, 3-(3,3-dimethyl-1-triazenyl)- (9CI) (CA INDEX NAME)



CC 25-5 (Noncondensed Aromatic Compounds)
IT 62-53-3, reactions 88-21-1 95-55-6 99-05-8 121-47-1 121-57-3 123-30-8 150-13-0 **591-27-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(diazotization of, in tetrafluoroboric acid and hexafluorophosphoric acid)

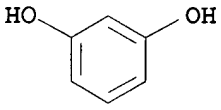
IT 118-92-3P 364-90-9P 369-57-3P 369-58-4P 369-61-9P
456-25-7P 659-44-9P 772-99-6P 836-69-1P 836-72-6P
2145-24-6P **7203-91-0P** **7227-91-0P**
7227-93-2P 14783-89-2P **20119-28-2P**
20241-07-0P 20873-47-6P **35433-91-1P**
37599-71-6P 39151-44-5P 39151-46-7P 39151-47-8P
39151-50-3P 39151-52-5P 39151-53-6P 39151-54-7P
39201-85-9P **39201-86-0P** 39948-22-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L67 ANSWER 30 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:40270 HCAPLUS
DOCUMENT NUMBER: 76:40270
TITLE: Two-component diazotype material
PATENT ASSIGNEE(S): Kalle A.-G.
SOURCE: Brit., 5 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

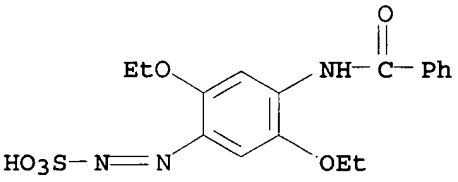
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1234244		19710603	GB <--	19680806
FR 1582204			FR	
PRIORITY APPLN. INFO.:			DE <--	19670808

GI For diagram(s), see printed CA Issue.
AB In a neg.-working diazotype copy process, esp. for neg. microfilm enlargements, the light sensitive layer contains a diazosulfonate, which has no basic N atom in the p-position to the diazo group, and a coupling agent. The imagewise exposed material is fixed by treatment with an aq. soln. of a nonvolatile acid having pH 1-4, esp. citric acid. Known 2,3-dihydroxy-naphthalene coupling agents are not suitable for the production of blue images. Suitable coupling agents are 2-hydroxy-3-naphthamides I, where R1 is a C1-6 polyhydroxyalkyl group or a hydroxyalkoxyalkyl group having up to C8, R2 is H or C1-6 hydroxyalkyl, and R3 is H, halogen or C1-4 alkoxy. Thus, a conventional photoprinting base paper was coated with a soln contg. 3.6 g Na 2,5-diethoxy-4-(benzoylamino)benzenediazo-sulfonate, 3 g caffeine, 4 ml 10% aq. NaOH, 6 g Na benzaldehyde-2-sulfonate, 3 ml glycerol, 0.2 g anionic wetting agent, 0.2 g Na2SO3.7H2O, 1.8 g 2-hydroxy-3-(β-hydroxyethylamidocarbonyl)naphthalene, 24 g acrylamide and 100 ml H2O. A 24X enlargement was prepd. on this paper from a neg. Ag film original having a photog. d. of 1.2 using a projector having a 500 W Hg lamp. A blue image of good contrast was produced in 30 sec. The image was fixed in a conventional wet developing app. with an aq. soln. contg. 12.5% citric acid, 5% ZnCl2 and 0.1% anionic wetting agent, followed by overall exposure to a uv lamp. The copy retained its blue on white image even after long storage.
IT **108-46-3**, properties

RL: USES (Uses)
(diazo process coupler from)
RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)

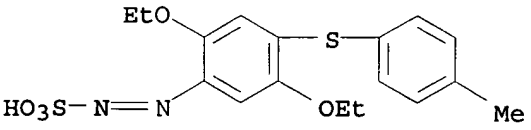


IT **36429-18-2 36429-19-3**
RL: USES (Uses)
(light-sensitive compns. contg., for neg.-working diazo process)
RN 36429-18-2 HCAPLUS
CN Diazenesulfonic acid, [4-(benzoylamino)-2,5-diethoxyphenyl]-, monosodium salt (9CI) (CA INDEX NAME)



● Na

RN 36429-19-3 HCAPLUS
CN Diazenesulfonic acid, [2,5-diethoxy-4-[(4-methylphenyl)thio]phenyl]-, sodium salt (9CI) (CA INDEX NAME)



● Na

IC G03C
CC 74 (Radiation Chemistry, Photochemistry, and Photographic Processes)
IT 92-80-8 **108-46-3**, properties 10000-54-1 10089-93-7
36429-23-9 36429-24-0
RL: USES (Uses)
(diazo process coupler from)
IT **36429-18-2 36429-19-3**
RL: USES (Uses)
(light-sensitive compns. contg., for neg.-working diazo process)

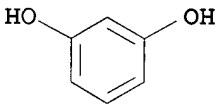
L67 ANSWER 31 OF 31 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1959:51679 HCAPLUS
DOCUMENT NUMBER: 53:51679
ORIGINAL REFERENCE NO.: 53:9357e-g
TITLE: Comparative study of the use of microorganisms in the screening of potential antitumor agents
AUTHOR(S): Foley, G. E.; McCarthy, R. E.; Binns, V. M.; Snell, E. E.; Guirard, B. M.; Kidder, G. W.; Dewey, V. C.; Thayer, P. S.
CORPORATE SOURCE: Children's Med. Center, Boston, MA
SOURCE: Annals of the New York Academy of Sciences (**1958**), 76, 413-41
CODEN: ANYAA9; ISSN: 0077-8923
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

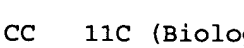
AB Collaborative studies were organized to include 16 microbial systems, with bacteria, fungi, and protozoa as the assay microorganisms. A series of 200 compds. were studied. It appears that 95% of the compds. adjudged to be tumor-active in animal assays can be detected by virtue of their inhibitory effects on microorganisms, with as few as 4 selected bioassay systems. 34 refs.

IT **108-46-3**, Resorcinol **7227-91-0**, Triazene, 3,3-dimethyl-1-phenyl-
(growth inhibition by)

RN 108-46-3 HCAPLUS
CN 1,3-Benzenediol (9CI) (CA INDEX NAME)



RN 7227-91-0 HCAPLUS
CN 1-Triazene, 3,3-dimethyl-1-phenyl- (9CI) (CA INDEX NAME)



CC 11C (Biological Chemistry: Microbiology)

IT 50-23-7, Cortisol 50-44-2, Purine-6-thiol 50-54-4, Quinidine, sulfate 51-17-2, Benzimidazole 51-28-5, Phenol, 2,4-dinitro- 51-79-6, Ethyl carbamate 53-79-2, Puromycin 54-11-5, Nicotine 54-62-6, Glutamic acid, N-[p-[[(2,4-diamino-6-pteridinyl)methyl]amino]benzoyl]- 55-98-1, Methanesulfonic acid, tetramethylene ester 56-75-7, Chloramphenicol 57-24-9, Strychnine 57-27-2, Morphine 58-08-2, Caffeine 58-14-0, Pyrimidine, 2,4-diamino-5-(p-chlorophenyl)-6-ethyl- 58-55-9, Theophylline 58-60-6, Adenosine, 3'-amino-3'-deoxy-N,N-dimethyl- 59-05-2, Glutamic acid, N-[p-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- 59-30-3, Folic acid 61-73-4, Methylene blue 65-45-2, Salicylamide 66-81-9, Glutarimide, 3-[2-(3,5-dimethyl-2-oxocyclohexyl)-2-hydroxyethyl]- 66-84-2, Glucosamine, hydrochloride 67-20-9, Hydantoin, 1-(5-nitrofurfurylideneamino)- 67-68-5, Methyl sulfoxide 75-12-7, Formamide 75-87-6, Chloral 78-38-6, Phosphonic acid, ethyl-, diethyl ester 78-46-6, Phosphonic acid, butyl-, dibutyl ester 79-16-3, Acetamide, N-methyl- 80-17-1, Benzenesulfonic

acid, hydrazide 83-25-0, Succinimide, N-phenyl- 83-67-0, Theobromine 87-66-1, Pyrogallol 88-88-0, Picryl chloride 94-52-0, Benzimidazole, 5(or 6)-nitro- 95-14-7, Benzotriazole 100-35-6, Triethylamine, 2-chloro- 106-48-9, Phenol, p-chloro- 107-94-8, Propionic acid, 3-chloro- 107-96-0, Propionic acid, 3-mercapto- 108-01-0, Ethanol, 2-dimethylamino- **108-46-3** , Resorcinol 109-12-6, Pyrimidine, 2-amino- 111-68-2, Heptylamine 111-77-3, Ethanol, 2-(2-methoxyethoxy)- 115-02-6, Serine, diazoacetate 119-30-2, Salicylic acid, 5-iodo- 120-67-2, Ethanol, 2-(2,4-dichlorophenoxy)- 120-83-2, Phenol, 2,4-dichloro- 121-53-9, Benzoic acid, m-sulfo- 121-66-4, Thiazole, 2-amino-5-nitro- 122-42-9, Carbanilic acid, isopropyl ester 123-39-7, Formamide, N-methyl- 124-68-5, 1-Propanol, 2-amino-2-methyl- 128-62-1, Narcotine 134-58-7, v-Triazolo[4,5-d]pyrimidin-7(6H)-one, 5-amino- 139-93-5, Arsphenamine 140-79-4, Piperazine, 1,4-dinitroso- 141-86-6, Pyridine, 2,6-diamino- 142-45-0, Acetylenedicarboxylic acid 148-24-3, 8-Quinolinol 148-51-6, 3-Pyridinemethanol, 5-hydroxy-4,6-dimethyl-, hydrochloride 314-19-2, Apomorphine, hydrochloride 316-41-6, Berberine, sulfate 350-03-8, Ketone, methyl 3-pyridyl 352-97-6, Glycocyamine 371-40-4, Aniline, p-fluoro- 477-30-5, Demecolcine 481-06-1, Santonin 485-71-2, Cinchonidine 497-59-6, Meconic acid 505-10-2, 1-Propanol, 3-(methylthio)- 538-03-4, Phenol, 2-amino-4-arsenoso-, hydrochloride 538-28-3, Pseudourea, 2-benzyl-2-thio-, hydrochloride 548-62-9, Crystal violet 553-24-2, Neutral red 561-20-6, Cacotheline 587-65-5, Acetanilide, 2-chloro- 598-55-0, Carbamic acid, methyl ester 609-85-8, Anthranilic acid, 3,5-dibromo- 619-80-7, Benzamide, p-nitro- 623-76-7, Urea, 1,3-diethyl- 625-56-9, Acetic acid, chloro-, methyl ester 628-83-1, Butane, 1-thiocyanato- 765-15-1, Dodecane, 1-thiocyanato- 850-57-7, Thebaine, hydrochloride 897-55-2, Quinoline, 4-(p-dimethylaminostyryl)- 924-42-5, Acrylamide, N-(hydroxymethyl)- 956-04-7, Chalcone, 4-chloro- 1011-92-3, Cinnamic acid, α-cyano- 1120-48-5, Dioctylamine 1420-53-7, Codeine, sulfate 1468-26-4, v-Triazolo[4,5-d]pyrimidine-5,7(4H,6H)dione 1571-33-1, Phosphonic acid, phenyl- 1696-20-4, Morpholine, 4-acetyl- 1759-53-1, Cyclopropanecarboxylic acid 2021-58-1, 2-Thiophenealanine 2051-95-8, Propionic acid, 3-benzoyl- 2150-48-3, Pyronine B 2545-84-8, Taurine, N-(2,4-dihydroxy-3,3-dimethylbutyryl)- 3054-70-4, 4-Pyrimidinol, 2,6-diamino-5-phenylazo- 3085-45-8, Ethanol, 2,2'-sulfinyldi- 3430-95-3, Lauranilide 3741-38-6, Ethylene sulfite 3891-07-4, Phthalimide, N-2-hydroxyethyl- 3915-61-5, Quinolinium, 2-(p-dimethylaminostyryl)-1-methyl-, iodide 4005-51-0, 1,3,4-Thiadiazole, 2-amino- 4248-77-5, Methanesulfonic acid, nonamethylene ester 4334-74-1, p-Anisaldehyde, thiosemicarbazone 4363-94-4, Cinchoninaldehyde, 6-methoxy- 4375-11-5, Imidodicarboxylic acid, dihydrazide 4491-22-9, Pyrrole-2-carboxamide, N-[5-[(2-carbamoylethyl)carbamoyl]-1-methylpyrrol-3-yl]-4-(2-guanidinoacetimidoylamino)-1-methyl-, hydrochloride 4514-52-7, s-Triazine, 4,6-diamino-1-(m-bromophenyl)-1,2-dihydro-2,2-dimethyl-, hydrochloride 4617-17-8, Ether, bis(2-thiocyanatoethyl) 4845-99-2, Brucine, sulfate 4887-82-5, 1H-Benzimidazole, 5-chloro- 5325-67-7, Propiophenone, 3-hydroxy-2-methyl-3-(2-pyridyl)- 5329-15-7, o-Acetanisidide, 4'-amino- 5329-33-9, Pseudourea, 2-methyl-, hydrochloride 5330-72-3, Pyrylium, 2,6-dimethyl-4-(phenacylthio)-, bromide 5332-73-0, Propylamine, 3-methoxy- 5338-14-7, 3-Pentanone, 2,4-dimethyl-, semicarbazone 5338-29-4, 4-Pyridazineacetic acid,

1,2,3,6-tetrahydro-3,6-dioxo-2-phenyl- 5349-55-3, Lactic acid, allyl ester 5393-55-5, 1,3,4-Thiadiazole, 2-acetamido- 5394-04-7, Acrylic acid, trichloro-, sodium salt 5395-03-9, Tyrosine, N-(2-carboxyethyl)-, L- 5397-34-2, Phenol, 2,4'-sulfonyldi- 5399-22-4, Lauric acid, hydrazide 5405-65-2, s-Triazine, 4-amino-6-p-chloroanilino-1,2-dihydro-2,2-dimethyl- 5405-66-3, s-Triazine, 4-amino-6-anilino-1,2-dihydro-2,2-dimethyl- 5423-04-1, Thebaine, tetrahydro-, hydrochloride 5735-19-3, Isoalloxazine, 7,8-dimethyl-10-D-galacto-2,3,4,5,6-pentahydroxyhexyl- 5943-04-4, Sulfone, chloromethyl p-chlorophenyl 5984-80-5, Isoalloxazine, 6,7-dimethyl-10-(D-ribo-2,3,4,5-tetrahydroxypentyl)- 6164-47-2, Protopine, hydrochloride 6333-47-7, s-Triazine, 4,6-diamino-1-(m-bromophenyl)-1,2-dihydro-2-undecyl-, hydrochloride 7182-80-1, Urea, amidino-, sulfate **7227-91-0**, Triazene, 3,3-dimethyl-1-phenyl- 10018-19-6, Cotarnine chloride 10124-50-2, Potassium arsenite 11005-63-3, Strophanthin 13073-35-3, Butyric acid, 2-amino-4-(ethylthio)- 13318-64-4, s-Triazine, 4,6-diamino-1-(3,4-dichlorophenyl)-1,2-dihydro-2,2-dimethyl-, hydrochloride 14150-71-1, Thiocyanic acid, 1,2-ethenediyl ester 14358-44-2, Quinine, hydrobromide 15521-77-4, 3-Pyridinesulfonic acid, sodium salt 15720-25-9, 4-Imidazolidinehexanoic acid, 5-methyl-2-oxo- 17711-82-9, s-Triazine, 4,6-diamino-1,2-dihydro-2,2-dimethyl-1-(2,6-xylyl)-, hydrochloride 18588-57-3, Pyrimidine, 2,4-diamino-5-(3,4-dichlorophenyl)-6-ethyl- 22592-41-2, Acetanilide, 4'-formyl-, semicarbazone 22665-47-0, Propyl thiopyrophosphate, (PrO)4P2O2S 23945-44-0, 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-2,4-dioxo- 26628-22-8, Sodium azide 31221-06-4, Barbituric acid, 5-diazo- 32014-70-3, Uracil, 5,6-diamino-, sulfate 34289-60-6, 2-Pyrimidinol, 4,6-dimethyl-, hydrochloride 54327-10-5, Methyl green 62697-73-8, Butyric acid, 2-amino-4-(methylsulfinyl)- 65591-11-9, v-Triazolo[4,5-d]pyrimidine, 5,7-diamino-, sulfate 77918-08-2, Diethylene glycol, dibenzenesulfonate 96432-94-9, Benzoic acid, p-(4,6-diamino-2,2-dimethyl-s-triazin-1(2H)-yl)-, hydrochloride 98954-13-3, Benzamide, p-(3-amidinoguanidino)- 99184-04-0, Carbonic acid, allyl p-chlorophenyl ester 101092-00-6, s-Triazine, 4-amino-6-anilino-1,2-dihydro-2-phenyl- 102466-49-9, Quinoline, 7-chloro-4-[(4-diethylamino-1-methylbutyl)amino]-3,6-dimethyl-, diphosphate 108676-72-8, Guanidine, 3-(6-chloro-4-methyl-2-quinazolinyl)-1,1-dimethyl-, nitrate 109732-05-0, Ammonium, (α,α-dimethylbenzyl)trimethyl-, iodide 110031-00-0, Succinic acid, ester with 10-(2-hydroxyethyl)-7,8-dimethylisoalloxazine 117122-07-3, 1,3,4-Thiadiazole, 2-(allylamino)-5-methyl-, hydrochloride 120089-34-1, 1,3,4-Thiadiazole, 2-ethylamino-, hydrochloride 122473-31-8, Pyridinium, 1-dodecyl-4-nonyl-, chloride 857173-03-6, Acridine, 9-[(3-dibutylaminopropyl)amino]-, phosphate 859916-25-9, Benzenesulfonic acid, ester with diethylene glycol
(growth inhibition by)

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